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MATHEMATICS

Transformed Point Arithmetic for Digital Computers

by

M. WARMUS

Presented by H. STEINHAUS on December 28, 1960

In many so-called fixed-point digital computers the arithmetical operations are carried out merely on numbers from the interval $(-1, +1)$. If dealing with numbers of widely varying size is necessary, we use what is called floating point subroutines. The following system may be considered to be classical.

Let us work in the binary system with n-bit words. We write each number $x \neq 0$ in the form

$$x = 2^p \cdot z,$$

where $1/2 \leqslant |z| < 1$ and p is an integer. The number p is called the exponent and the number z the mantissa of the number x. We divide the word of the machine into 2 parts. We code the exponent in the first and the mantissa in the second part of the word. Thus a subroutine for floating point arithmetical operations consists of: separation of the exponent from the mantissa, calculation of the exponent and, separately, of the mantissa of the result and formation of the result in a single word of the machine.

Another solution of the problem of the floating point was given by A. B. Empacher [1]. His idea led us to a new solution, which is presented in this paper.

We may consider the problem of floating point arithmetic as the problem of such a transformation of the interval $(-\infty, +\infty)$ into the interval $(-1, +1)$, by which arithmetical operations on numbers from the interval $(-\infty, +\infty)$ correspond to such operations on their transforms from the interval $(-1, +1)$, which are easy to be performed in the machine. E.g., let $O(X, Y) = Z$ be the operation corresponding to a given operation $o(x, y) = z$, where x, y, z belong to the interval $(-\infty, +\infty)$ and X, Y, Z are their transforms from the interval $(-1, +1)$. Let us suppose, that the transformation is defined by the function $X = f(x)$, which has an inverse function $x = F(X)$. Then we have

$$O(X, Y) = f[o(x, y)] = f[o(F(X), F(Y))]. \tag{1}$$

I propose the following transformation:

$$X = \frac{ax}{1+|x|} = f(x), \tag{2}$$

where a is an arbitrary constant from the interval $(-1, +1)$, usually very close to 1. Thus we have

$$x = \frac{X}{a - |X|} = F(X) \tag{3}$$

and

$$-a < X < a. \tag{4}$$

Let X and Y denote the transforms of the numbers x, y, respectively, by the transformation (2). Moreover, let $X \hat{+} Y$, $X \hat{-} Y$, $X \hat{\cdot} Y$, $X \hat{:} Y$ denote the operations on numbers X, Y corresponding to the operations $x+y$, $x-y$, xy, x/y, respectively.

Taking into account that by (4)

$$a - |X| > 0, \quad a - |Y| > 0 \tag{5}$$

and introducing the notation

$$\overline{|X|} = a - |X|, \tag{6}$$

we obtain

$$\begin{cases} X \hat{+} Y = \dfrac{aZ}{\overline{|X|}\,\overline{|Y|} + |Z|}, & \text{where } Z = X\overline{|Y|} + Y\overline{|X|}, \\ X \hat{-} Y = X \hat{+} (-Y), \\ X \hat{\cdot} Y = \dfrac{aZ}{\overline{|X|}\,\overline{|Y|} + |Z|}, & \text{where } Z = XY, \\ X \hat{:} Y = X \hat{\cdot} \overline{|Y|}\ \operatorname{sgn} Y, & Y \neq 0. \end{cases} \tag{7}$$

The operations (7) are performable in a fixed-point machine, because — what is easily proved — we have

$$|X| < a < 1, \quad |Y| < a < 1,$$

$$0 < \overline{|X|} \leqslant a < 1, \quad 0 < \overline{|Y|} \leqslant a < 1,$$

$$|XY| < a^2 < 1, \quad |X|\,\overline{|Y|} < a^2 < 1, \quad \overline{|X|}\,|Y| < a^2 < 1, \quad \overline{|X|}\,\overline{|Y|} \leqslant a^2 < 1,$$

$$\left| X\overline{|Y|} + Y\overline{|X|} \right| < a^2 < 1, \quad a\left| X\overline{|Y|} + Y\overline{|X|} \right| < a^3 < 1,$$

$$\overline{|X|}\,\overline{|Y|} + \left| X\overline{|Y|} + Y\overline{|X|} \right| \leqslant a^2 < 1,$$

$$|a\,XY| < a^3 < 1, \quad \overline{|X|}\,\overline{|Y|} + |XY| \leqslant a^2 < 1,$$

and by (1), (2), and (4)

$$|X \hat{+} Y| < a < 1, \quad |X \hat{-} Y| < a < 1, \quad |X \hat{\cdot} Y| < a < 1, \quad |X \hat{:} Y| < a < 1.$$

It is worth mentioning, that, if X is the transform of x by the transformation (2), then $-x$ has the transform $-X$ and $1/x$ the transform $a \operatorname{sgn} X - X = \operatorname{sgn} X \cdot \overline{|X|}$.

The whole subroutine of the operations (7) is several times shorter than the corresponding one for classical floating-point operations. Moreover, we avoid the difficulties connected with introduction of zero in the classical floating-point system. The relative error of results obtained by means of the operations (7) has an unique minimum for $|x| = 1$, by the assumption that the absolute error of numbers X is constant. This results from the formula

$$\varepsilon(x) = \frac{dx}{|x|} = y\,dX, \tag{8}$$

where

$$y = \frac{(1+|x|)^2}{|x|}, \tag{9}$$

which is obtained from (2). Namely, the function (9) has an unique minimum at $|x| = 1$.

It results from (8) and (9) that

$$\varepsilon\left(\frac{1}{x}\right) = \varepsilon(x)$$

and

$$\lim_{x \to \pm\infty} \varepsilon(x) = \infty, \qquad \lim_{x \to 0} \varepsilon(x) = \infty.$$

Taking into account that in the classical system the relative error is approximatively constant, but in each word we must lose some bits for the exponent, it is seen that we calculate in the proposed system with greater precision than in the classical one if we use numbers close to 1, and with less precision if the absolute values are either very great or very small. Moreover, we must also take into account that in the classical system very often the great precision is only illusory, e.g. after the subtraction of two numbers, little differing from each other.

It is possible to construct such computers, for which (7) would be built-in floating-point operations.

I propose to call the system described above the transformed-point system.

The transformed-point system often enables us to solve some problems in a new way: instead of transforming single operations we transform whole formulas or equations. This method will be described in a separate paper.

Finally, for illustration of the economy of the proposed transformed-point system, it may be mentioned, that in the Polish computer EMAL-2 the whole subroutine for all arithmetical operations consists of 163 instructions in the classical and of 56 instructions in the transformed-point system.

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MATHEMATICS

Approximations and Inequalities in the Calculus of Approximations. Classification of Approximate Numbers

by

M. WARMUS

Presented by H. STEINHAUS on December 28, 1960

This note is a continuation of [1], in which a definition of the relation of approximation between two approximate numbers was given. However, a change of denotation appeared to be suitable. Namely, if the approximate number $\overset{b}{B}$ approximates the approximate number $\overset{a}{A}$, i.e. if

$$b - a \geqslant |B - A|,$$

we shall write

$$\overset{a}{A} \subseteq \overset{b}{B} \text{ or } \overset{b}{B} \supseteq \overset{a}{A}. \tag{1}$$

(In the paper just quoted the denotation $\Rightarrow$ was used instead of $\subseteq$).

We now introduce several new definitions, which are necessary for further applications of the calculus of approximations. From now on by numbers we shall mean approximate numbers.

We say that the number $\overset{b}{B}$ approximates sharply the number $\overset{a}{A}$ and we write

$$\overset{a}{A} \subset \overset{b}{B} \text{ or } \overset{b}{B} \supset \overset{a}{A}, \tag{2}$$

if and only if

$$b - a > |B - A|. \tag{3}$$

Sometimes for the sake of distinction we say in the case (1) that the number $\overset{b}{B}$ approximates weakly the number $\overset{a}{A}$.

We say that the number $\overset{a}{A}$ is less (i.e. weakly less), sharply less, greater (i.e. weakly greater), sharply greater than the number $\overset{b}{B}$ and we write

$$\overset{a}{A} \leqslant \overset{b}{B}, \quad \overset{a}{A} < \overset{b}{B}, \quad \overset{a}{A} \geqslant \overset{b}{B}, \quad \overset{a}{A} > \overset{b}{B}, \tag{4}$$

respectively, if and only if the corresponding inequality

$$(5)\qquad \begin{cases} B - A \geqslant |b - a|, \\ B - A > |b - a|, \\ A - B \geqslant |a - b|, \\ A - B > |a - b|, \end{cases}$$

holds.

With respect to isomorphism of the set of numbers $\overset{0}{A}$ to the set of real numbers, we may consider (4) as a generalization of common inequalities between real numbers.

Similarly as it was convenient to reduce approximations (and thus also sharp approximations) to the following two rules

$$\text{the rounding-off rule:} \quad \overset{a}{A} + c \subseteq \overset{a+|c|}{A};$$

$$\text{the extending rule:} \quad \overset{a}{A} \subseteq \overset{b}{A} \quad \text{if} \quad b \geqslant a,$$

so it is also convenient to reduce inequalities (4) to the rounding-off rule and to the increasing rule, which is defined as follows:

$$\overset{a}{A} \leqslant \overset{a}{B} \quad \text{if} \quad A \leqslant B.$$

Definitions of approximations and inequalities enable us to introduce the following classification of approximate numbers.

Numbers greater (i.e. weakly greater) than zero are called positive, numbers less (i.e. weakly less) than zero are called negative. Positive and negative numbers are called signed numbers.

Numbers approximating (i.e. weakly approximating) zero are called over-zero numbers, numbers approximated by zero are called under-zero numbers. Over-zero and under-zero numbers are called mixed numbers.

In a similar way we introduce sharply positive and sharply negative numbers, sharply signed numbers, sharply over- and under-zero numbers, sharply mixed numbers.

The number $\overset{a}{A}$ is a divisor of zero if and only if $|A| = |a|$. Then it is called a zero-number. A zero-number $\overset{a}{A}$ is positive (if $A \geqslant 0$) or negative (if $A \leqslant 0$), it is also an over-zero (if $a \geqslant 0$) or an under-zero (if $a \leqslant 0$) number. If we write a zero-number $\overset{a}{A}$ in the form $[A - a, A + a]$, we have $A - a = 0$ or $A + a = 0$. Thus, every zero-number $\overset{a}{A}$ can be written in the form $[0, 2A]$ or $[2A, 0]$. In the first case it is called a left zero-number, in the second case it is called a right zero-number. We see that left zero-numbers are positive over-zero or negative under-zero numbers and right zero-numbers are positive under-zero or negative over-zero numbers.

If we represent a number $\overset{x}{X}$ by a point in a plane with the rectangular Cartesian co-ordinates (X, x), we may illustrate the just introduced classification of approximate numbers by the Fig. 1.

The horizontally lined part of the plane corresponds to the set of all signed numbers. The vertically lined part corresponds to the set of all mixed numbers.

If we represent the number $\overset{x}{X} = [y, Y]$ by a point in a plane with the rectangular Cartesian co-ordinates (y, Y), we obtain the illustration given by the Fig. 2.

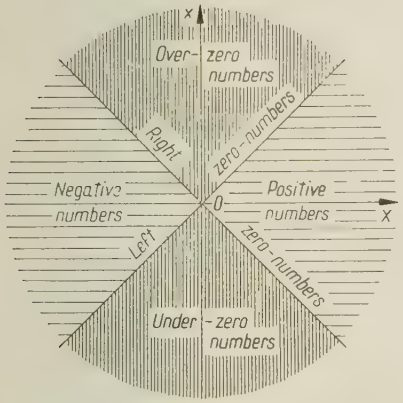

Fig. 1.

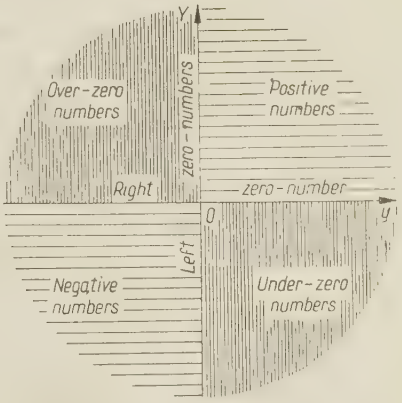

Fig. 2.

Sharply positive, sharply negative, sharply signed, sharply over- and under-zero numbers, sharply mixed numbers are, respectively, positive, negative, signed, over- or under-zero numbers, mixed numbers, which are not zero-numbers.

The numbers $\overset{a}{A}$ and $(\overset{-a}{-A})$ are called opposite.

Thus, we see, that $A = [b, B]$ is:

(6)

a positive	number if and only if	$A \geqslant \lvert a\rvert$, i.e. $b \geqslant 0;\ B \geqslant 0,$
a sharply positive	,, ,, ,, ,, ,,	$A > \lvert a\rvert$, ,, $b > 0;\ B > 0,$
a negative	,, ,, ,, ,, ,,	$A \leqslant -\lvert a\rvert$, ,, $b \leqslant 0;\ B \leqslant 0,$
a sharply negative	,, ,, ,, ,, ,,	$A < -\lvert a\rvert$, ,, $b < 0;\ B < 0,$
a signed	,, ,, ,, ,, ,,	$\lvert A\rvert \geqslant \lvert a\rvert$, ,, $bB \geqslant 0,$
a sharply signed	,, ,, ,, ,, ,,	$\lvert A\rvert > \lvert a\rvert$, ,, $bB > 0,$
an over-zero	,, ,, ,, ,, ,,	$\lvert A\rvert \leqslant a$, ,, $b \leqslant 0;\ B \geqslant 0,$
a sharply over-zero	,, ,, ,, ,, ,,	$\lvert A\rvert < a$, ,, $b < 0;\ B > 0,$
an under-zero	,, ,, ,, ,, ,,	$-\lvert A\rvert \geqslant a$, ,, $b \geqslant 0;\ B \leqslant 0,$
a sharply under-zero	,, ,, ,, ,, ,,	$-\lvert A\rvert > a$, ,, $b > 0;\ B < 0,$
a mixed	,, ,, ,, ,, ,,	$\lvert A\rvert \leqslant \lvert a\rvert$, ,, $bB \leqslant 0,$
a sharply mixed	,, ,, ,, ,, ,,	$\lvert A\rvert < \lvert a\rvert$, ,, $bB < 0,$
a zero-	,, ,, ,, ,, ,,	$\lvert A\rvert = \lvert a\rvert$, ,, $bB = 0,$
a left zero-	,, ,, ,, ,, ,,	$A = a$, ,, $b = 0,$
a right zero-	,, ,, ,, ,, ,,	$A = -a$, ,, $B = 0.$

The above introduced classification will facilitate the formulation of some theorems concerning approximations and inequalities. But first of all we give several theorems following immediately from this classification and the definitions of arithmetical operations given in the previous paper. From now on by operations we shall mean regular operations.

The sum of two positive, negative, over- or under-zero numbers is also a positive, negative, over- or under-zero number, respectively. If, moreover, at least one of those numbers is a sharply positive, sharply negative, sharply over- or under-zero number, respectively, so is the sum.

Subtraction is equivalent to addition of the opposite number.

The product of two numbers equals zero if and only if one of them is zero, or, one of them is a left zero-number and the other is a right zero-number. The product of two numbers is a zero-number, if and only if at least one of them is a zero-number. Thus, the product of two numbers, which are not zero-numbers, is not a zero-number.

The product of two positive numbers is also positive. The product of a sharply positive number and a positive one is positive. The product of two sharply positive numbers is also sharply positive.

We obtain easily the rules for other cases, when we make account of the fact, that every negative, over- or under-zero number may be considered as the product $\alpha\cdot(-1)$, $\alpha\Lambda$, $\alpha\cdot(-\Lambda)$, respectively, where α is a positive number and $\Lambda = 0^{\frac{1}{1^2}}$ $(1^2 = 1)$. For example, when we multiply a negative number and an under-zero one, we consider them as the products $\alpha\cdot(-1)$ and $\beta\cdot(-\Lambda)$, where α and β are positive, and thus we obtain $(\alpha\beta)\cdot\Lambda$, i.e. an over-zero number. When we multiply a sharply over-zero number and an under-zero one, then considering them as the products $\alpha\cdot\Lambda$ and $\beta\cdot(-\Lambda)$, where α is sharply positive and β positive, we obtain the product $(\alpha\beta)\cdot(-1)$, which is a negative number.

In a similar way we obtain the rules for division, taking into account that a divisor can not be a zero-number and $1/\Lambda = \Lambda$. If, for example, we divide a sharply negative number by a sharply under-zero one, then considering them as the products $\alpha\cdot(-1)$ and $\beta\cdot(-\Lambda)$, where α and β are sharply positive, we obtain the quotient in the form $\frac{\alpha}{\beta}\cdot\frac{1}{\Lambda} = \frac{\alpha}{\beta}\Lambda$ as a sharply over-zero number. Here we have made account of the rule, that the quotient of two sharply positive numbers is also sharply positive, and the quotient of a positive number by a sharply positive one is positive.

We now pass to the rules of operations on approximations and inequalities. These rules follow immediately from the definitions of those relations.

We call the relations

(7) $\subseteq$ and $\supseteq$, $\subset$ and $\supset$, $\leqslant$ and $\geqslant$, $<$ and $>$,

opposite; the relations

(8) $\subseteq$ and $\leqslant$, $\subset$ and $<$, $\supseteq$ and $\geqslant$, $\supset$ and $>$,

adjoint; the relations

(9) $\subseteq$ and $\geqslant$, $\subset$ and $>$, $\supseteq$ and $\leqslant$, $\supset$ and $<$,

opposite-adjoint. The relations $\subseteq$, $\supseteq$, $\leqslant$, $\geqslant$, are called weak and the relations $\subset$, $\supset$, $<$, $>$, are called sharp. A passing from $\subset$ to $\subseteq$, from $\supset$ to $\supseteq$, from $<$ to $\leqslant$, or from $>$ to $\geqslant$, is called a weakening of the relation.

We now have the following theorems:

An arbitrary number may be added or subtracted on the both sides of an approximation or inequality. (It follows that an arbitrary number may be "shifted" from one side of an approximation or inequality to the other with alteration into the opposite one).

Approximations and inequalities may be multiplied or divided on both sides by an arbitrary, sharply positive number.

Weak approximations and weak inequalities may be multiplied on both sides by an arbitrary positive number.

If we multiply a sharp approximation or a sharp inequality on both sides by a positive number, we weaken the relation.

Approximations and inequalities may be multiplied or divided on both sides by an arbitrary sharply negative, sharply over-or under- zero number with alteration of the relation into the opposite, adjoint, or opposite-adjoint one, respectively.

Weak approximations and weak inequalities may be multiplied on both sides by an arbitrary negative, over- or under-zero number with alteration of the relation into the opposite, adjoint, opposite-adjoint one, respectively.

If we multiply a sharp approximation or a sharp inequality on both sides by a negative, over- or under-zero number, we weaken the relation and we must change it into the opposite, adjoint, opposite- adjoint one, respectively.

We leave out the simple proof of these theorems.

Finally, we present as an example the solution of the relation

$$\overset{-3}{1}\cdot\xi+(\overset{2}{-4})\supset 0.$$

"Shifting" the number $(\overset{2}{-4})$ to the other side of the approximation we have

$$\overset{-3}{1}\cdot\xi\supset\overset{-2}{4}.$$

Dividing the both sides by the sharply under-zero number $\overset{-3}{1}$ we obtain the result

$$\xi<\overset{-1.25}{0.25}=0.25-1.25\ A.$$

Similar operations will be used in further applications.

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MATHEMATICS

On Almost Realcompact Spaces

by
Z. FROLÍK

Presented by K. KURATOWSKI on February 7, 1961

It is well-known that a completely regular space is realcompact (see [4]: in the original terminology of E. Hewitt [5] realcompact spaces are called Q-spaces) if and only if the following condition is fulfilled:

(1) If the intersection of a maximal centred family $\mathfrak{z}$ of zerosets in P is empty, then the intersection of some countable subfamily of $\mathfrak{z}$ is empty.

In the present note we shall investigate a class of spaces closely connected to realcompact spaces.

DEFINITION. A space P will be called *almost realcompact*, if the following condition is fulfilled:

(2) *If $\mathfrak{A}$ is a maximal centred family of open sets and if $\overline{\mathfrak{A}}$ has the countable intersection property, then $\cap \overline{\mathfrak{A}} \neq \emptyset$.*

Notation and terminology

All spaces under consideration are supposed to be completely regular. If $\mathfrak{A}$ is a family of subsets of a space P and $R \subset P$, then

$$\mathfrak{A} \cap R = \{A \cap R;\ A \in \mathfrak{A}\}$$

$$U\,\mathfrak{A} = U\,\{A;\ A \in \mathfrak{A}\}$$

$$\overline{\mathfrak{A}}^P = \{A^P;\ A \in \mathfrak{A}\}$$

Of course, A^P or merely A, will be used to denote the closure of A in P. A centred family is a family with the finite intersection property. A family $\mathfrak{A}$ of sets has the countable intersection property, if the intersection of every countable subfamily of $\mathfrak{A}$ is non-void. A subset M of a space P will be called regular closed if $M = \operatorname{int} M$.

General concept of completeness

DEFINITION 2. Let $\alpha = \{\mathfrak{A}\}$ be a collection of coverings of a space P (not necessarily open). A α-Cauchy family is a centred family $\mathfrak{M}$ of subsets of P such that for every $\mathfrak{A}$ in α there exist an A in $\mathfrak{A}$ and an M in $\mathfrak{M}$ with $M \subset A$. The collection α will be called complete if $\cap \overline{\mathfrak{M}} \neq \emptyset$ for every α-Cauchy family $\mathfrak{M}$.

Example 1. An uniformity is complete if and only if the collection of all uniform coverings is complete.

Example 2. A space P is topologically complete in the sense of E. Čech, i.e. P is a G_δ in βP, if and only if there exists a complete countable collection of open coverings of P (for proof and further information see [1] and [2]).

Example 3. A space P is realcompact if and only if the collection ζ of all countable coverings of P consisting of zerosets is complete. First let us suppose that ζ is complete. Let $\mathfrak{z}$ be a maximal centred family of zerosets and let $\mathfrak{z}$ have the countable intersection property. It is easy to see that $\mathfrak{z}$ is ζ-Cauchy family. Indeed, supposing $\mathfrak{z} \cap \mathfrak{A} = \emptyset$ for some $\mathfrak{A}$ in ζ we can choose for every A in $\mathfrak{A}$ a $Z(A)$ in $\mathfrak{z}$ with $A \cap Z(A) = \emptyset$. Thus

$$\cap \{Z(A);\ A \in \mathfrak{A}\} \subset P - \cup \mathfrak{A} = \emptyset$$

which contradicts to countable intersection property of $\mathfrak{z}$. It follows that $\cap \mathfrak{z} \neq \emptyset$ and P is realcompact. Conversely, let us suppose that P is a realcompact space. Let $\mathfrak{M}$ be a ζ-Cauchy family. Without a loss of generality we may assume that $\mathfrak{M}$ is a maximal centred family. Let $\mathfrak{z}$ be the family of all zerosets in $\mathfrak{M}$. P being completely regular, we have $\cap \overline{\mathfrak{M}} = \cap \mathfrak{z}$. Thus it is sufficient to prove that $\mathfrak{z}$ has the countable intersection property. But this is obvious.

Theorem 1. *A space P is almost realcompact if and only if the collection γ of all countable open coverings of P is complete.*

The Proof of theorem 1 is an immediate consequence of the following simple

Lemma 1. *Let γ be the collection of all countable open coverings of a space P. A maximal centred family $\mathfrak{M}$ of open subsets of P is a γ-Cauchy family if and only if $\mathfrak{M}$ has the countable intersection property.*

The Proof of Lemma 1 is quite standard and may be left to the reader. The proof of Theorem 1 is analoguous to that from Example 3.

It is well-known that a space P is realcompact if and only if the uniformity $\mathcal{U}$ generated by the family of all realvalued continuous functions is complete. The collection η of all countable normal open coverings of P is a base for the family of all $\mathcal{U}$-uniform coverings. Thus, $\mathcal{U}$ is complete if and only if η is complete in the sense of Definition 1. Since η is contained in γ (See Theorem 1), we have at once from Theorem 1

Theorem 2. *Every realcompact space is almost realcompact.*

Note 1. Theorem 2 is an immediate consequence of the following theorem from [3]: For every realvalued continuous function f in a space P put

$$\mathfrak{N}(f) = \{\{x;\ |f(x)| < n\};\ n = 1, 2, \ldots\}.$$

The space P is realcompact if, and only if, the collection of all $\mathfrak{N}(f)$ is complete in the sense of Definition 1.

A mapping from a space P in a space Q will be called *perfect*, if f is continuous and closed mapping and the inverses of points are compact.

THEOREM 3. *If f is a perfect mapping from a space P onto a space Q, then P is almost realcompact if and only if Q is so.*

Proof. If Q is almost realcompact, then the collection $\gamma(Q)$ of all countable open coverings of Q is complete. It is easy to see that the collection $f^{-1}[\gamma(Q)]$ consisting of inverse images of $\mathfrak{A} \in \gamma(Q)$ is complete. Since

$$f^{-1}[\gamma(Q)] \subset \gamma(P)$$

we have that $\gamma(P)$ is complete and P is almost realcompact.

Conversely, let P be almost realcompact and hence $\gamma(P)$ be complete. It is easy to see that the collection δ of all countable coverings of P of the from $\{U_n\}$, $U_n \subset U_{nx_i}$, is complete, too. For every $\mathfrak{A}$ in δ, let $\mathfrak{A}'$ be the family of subsets of Q of the form

$$Q - f[P - A],$$

where A is running over all $A \in \mathfrak{A}$. The mapping f being perfect, every $\mathfrak{A}'$ is a countable open covering of P. It is easy to see that the collection of all $\mathfrak{A}'$, where $\mathfrak{A}$ runs over all $\mathfrak{A} \in \delta$, is complete. Thus Q is a realcompact space.

LEMMA 2. *Let a complete collection α of open coverings of a space P possess the following property: for every $\mathfrak{A}$ in α there exists a $\mathfrak{U}$ in α such that every B in $\mathfrak{U}$ is completely separated from some $P - A$ where $A \in \mathfrak{A}$. Then*

$$\cap \{\cup \overline{\mathfrak{A}}^{\beta P}; \mathfrak{A} \in \alpha\} = P.$$

Proof. The left side of the above equality will be denoted by R. Clearly, $R \supset P$. Let us suppose that there exists a point x in $R - P$. Let $\mathfrak{M}$ be the family of all open neighborhoods of x in βP and let $\mathfrak{N} = \mathfrak{M} \cap P$. It is easy to see that $\mathfrak{N}$ is a α-Cauchy family. Indeed, let $\mathfrak{A} \in \alpha$. Choose $\mathfrak{U}$ in α from Lemma 2. There exists a B in $\mathfrak{U}$ with $x \in B_{P\beta}$. If $A \in \mathfrak{A}$ is such that B and $P - A$ are completely separated, then $A \in \mathfrak{N} \cdot \alpha$ being a complete collection, we have

$$\cap \overline{\mathfrak{N}}^P = \emptyset,$$

but this is impossible since

$$\cap \overline{\mathfrak{N}}^P \subset \cap \overline{\mathfrak{M}}^{\beta P} = (x) \subset \beta P - P.$$

This contradiction completes the proof.

If P is a normal space, then for every $\mathfrak{A}$ in $\gamma(P)$ there exists a $\mathfrak{U}$ in $\gamma(P)$ satisfying the condition of Lemma 2, i.e. $\mathfrak{U}$ refines $\mathfrak{A}$. It follows that if P is a normal almost realcompact space, then

$$P = \cap \{\cup \mathfrak{A}; \mathfrak{A}^{\beta P} \in \gamma(P)\}.$$

The spaces of the form $\cup \mathfrak{A}^{\beta}$ are σ-compact. Thus every normal almost realcompact space is an intersection of σ-compact subspaces of βP, and consequently, P is realcompact. Thus we have proved

THEOREM 4. *Every normal almost realcompact space is realcompact.*

Combining Theorems 3 and 4 we obtain at once

THEOREM 5. *The image of a normal realcompact space under perfect mapping is a realcompact space.*

Note 2. It is obvious that the image of a realcompact (not necessarily normal) space under an open perfect mapping is a realcompact space. I do not know, whether the assumption of normality in Theorem 5 may be omitted.

We conclude this note by the following

THEOREM 6. *A normal space P is realcompact if and only if the collection φ of all countable closed coverings is complete.*

Note 3. If P is a countably paracompact space, then a maximal centred family $\mathfrak{E}$ of closed subsets of P is a $\varphi(P)$-Cauchy family if and only if $\mathfrak{E}$ has the countable intersection property. Thus a countably paracompact space is realcompact if, and only if, the intersection of maximal centred family $\mathfrak{E}$ of closed subsets is non-void, provided that $\mathfrak{E}$ has the countable intersection property.

Note 4. Let us consider the following condition (V) on a space P: If $\mathfrak{E}$ is a maximal centred family of closed sets and if $\mathfrak{E}$ does not have the countable intersection property, then there exist $F_n \in \mathfrak{E}$ and open sets U_n such that $U_n \supset F_n$ and $\bigcap_{n=1}^{\infty} U_n = \emptyset$.

Every countably paracompact space has the property (V). I do not know whether every normal space P with property (V) is countably paracompact.

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MATHEMATIQUE

Proprieté limite de la matrice du potentiel généralisé de simple couche du système parabolique d'équations

par

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Présenté par A. ZYGMUND le 10 février 1961

Il a été démontré dans les travaux antérieurs [1] que la limite du potentiel généralisé [2] de simple couche de l'équation parabolique normale aux dérivées partielles [3] converge, avec le temps $t \to \infty$, vers le potentiel de la densité limite d'une équation élliptique. Cette équation élliptique est dite limite, car ses coefficients constituent les limites des coefficients correspondants de l'équation parabolique. Le système parabolique d'équations aux dérivées partielles étant résolu dans les travaux [4], [5] pour les conditions très générales, et la matrice de ses solutions étant examinée dans [6], il est tout indiqué de poser le même problème limite pour cette matrice. Cependant, il se présente la difficulté suivante: la matrice des solutions du système élliptique n'était pas connue pour les conditions de même degré de généralité, [7], [8]. Nous allons trouver cette matrice dans la présente communication en intégrant formellement la solution du système parabolique et en démontrant la légitimité du procédé en question.

Nous allons démontrer en plus que *la limite pour $t \to \infty$ du potentiel généralisé de simple couche du système parabolique d'équations est le potentiel généralisé, de densité limite, du système élliptique d'équations limites.*

Les hypothèses admises sont une simple application des hypothèses de la note [1]. Dans la note que voici, nous examinons seulement le cas où M (l'ordre du système) n'atteint pas n — la dimension de l'espace E, $(M < n)$*). Le cas de $M \geqslant n$ fût traité par Eidelman, [8], pour un système parabolique spécial, mais sa méthode s'applique aussi bien au cas général.

Soit dit que la solution du système élliptique d'équations donnée ci-dessous n'est pas encore entièrement satisfaisante. Notamment, le noyau résolvant de cette solution n'est convergent que dans un domaine restreint (voir l'hypothèse III)**). Il semble qu'on pourrait arriver à de meilleurs résultats en étudiant ce noyau directement.

*) Dans [1] on avait $M = 2$ et $n > 2$.

**) C'est aussi le cas de [1].

1. Nous allons nous servir de notations suivantes:

E — l'espace euclidien à n dimensions, ses points: $X = X(x_1, ..., x_n)$; $Y = Y(y_1, ..., y_n)$ etc.; t — le temps non négatif; Ω — un domaine de E; $\bar{\Omega}$ — la fermeture de Ω; Ω' — une région de E contenant $\bar{\Omega}$; c, C, C_0, C° — les constantes positives; $M < n$ — l'ordre du système parabolique d'équations linéaires, normales aux dérivées partielles; $k_1, ..., k_n$ — les composants entiers, non négatifs de chaque entier non négatif m ne surpassant pas M. On a notamment: $0 \leqslant k_i \leqslant m$; $k_1 + ... + k_n = m$; $0 \leqslant m \leqslant M < n$. Nous posons $(k_1, ..., k_n) = (\varkappa)$. Cela admis, les coefficients du système seront:

$$A_{\alpha\beta}^{k_1 ... k_n}(X,t) = A_{\alpha\beta}^{(\varkappa)}(X,t) \text{ et } D^m(u) = \partial^m u / \partial x_1^{k_1} ... \partial x_n^{k_n},$$

La matrice $\{u_{ij}\}_{i,j=1,...,N}$ des solutions du système sera nommée [u] et dès lors nous écrirons le système sous la forme

$$(1,1) \quad \hat{\psi}^{(\alpha)}(u) = \sum_{1 \leqslant j \leqslant N}^{0 \leqslant m \leqslant M} A_{\alpha j}^{(\varkappa)}(X,t) D^m(u_j) - \partial u_\alpha / \partial t \equiv 0, \alpha = 1, ... N, X \in \Omega, t > 0.$$

la somme étant répandue sur toute les suites $(\varkappa)$.

Si pourtant on désigne par P le nombre des composants de la somme (1,1) et si l'on pose $(a \cdot b)_1^P = (a_1 b_1 + ... + a_P b_P)$, on peut écrire le système (1,1) sous une forme encore plus abrégée:

$$(1',1) \quad \hat{\psi}^{(\alpha)}(u) = (A_\alpha(X,t) \cdot D(u))_1^P - \partial u_\alpha / \partial t \equiv 0, \quad \alpha = 1, ... N, X \in \Omega, t > 0.$$

Les hypothèses que nous allons admettre sont les suivantes:

I. Les coefficients du système (1,1) sont continus et bornés dans la région Ω' pour $t \geqslant 0$; ils sont soumis aux conditions d'Hölder:

$$(2,1) \quad |A_{\alpha j}^{(\varkappa)}(X,t) - A_{\alpha j}^{(\varkappa)}(X_1, t_1)| \leqslant \begin{cases} C_0 [|XX_1|^h + |t - t_1|^{h'}], m = M \\ C^0 |XX_1|^h, m < M, t = t_1 \end{cases}$$

$|X X_1|$ désigne la distance des points X et X_1 entre eux, h et h' sont constants et $0 < h \leqslant 1$; $0 < h' \leqslant 1$; nous posons $h_1 = \min(h, 2h')$.

On admet aussi que les limites:

$$(2',1) \quad \lim_{t \to 0} A_{\alpha j}^{(\varkappa)}(X,t) = \hat{A}_{\alpha j}(X), X \in \Omega', \alpha, j = 1, ... N$$

existent uniformément dans Ω' pour chaque suite $(\varkappa)$ définie ci-dessus.

II. Le système (1,1) est uniformément parabolique par rapport à la variable t dans la région Ω', au sens de Petrovsky, [4], (voir aussi [5], formules (5) à (7)). Il en résulte que le système d'équations:

$$(3,1) \quad \hat{\hat{\psi}}^{(\alpha)}(\hat{u}) = (\hat{A}_\alpha(X) \cdot D(\hat{u}))_1^P - \partial \hat{u}_\alpha / \partial t \equiv 0, \alpha = 1, ..., N$$

sera aussi parabolique au sens de Petrovsky dans le domaine Ω', pour $t > 0$. Nous allons transcrire la définition de la matrice des quasi-solutions [W] du système (1,1), donnée par W. Pogorzelski, [5], en ayant récours aux définitions formulées dans ce paragraphe, comme suit:

$$(4,1)\qquad W_{\alpha\beta}^{Z_2\xi} = W_{\alpha\beta}^{Z_2\xi}(X, t; Y, \tau) = (2\pi)^{-n}\int_{-\infty}^{+\infty} v_\alpha^\beta(t, \tau; Z, \xi; (s))\ \exp\ i(s\cdot(x-y))\,dS$$

$(s) = (s_1, ..., s_n); dS = ds_1 ... ds_n; (s(x-y)) = |(s_\nu(x_\nu - y_\nu))_1^n$ avec $s^2 = s_1^2 + ... + s_n^2$ on a:

$$(4',1)\qquad v_\alpha^\beta = v_\alpha^\beta(t, \tau; Z, \xi; (s)) = \sum_{\nu=1}^{N_1}(K_{\alpha\nu l}^\beta \cdot s^{Ml}(t-\tau)^l)_{l=0}^{\mu\nu} \exp \lambda'_\nu s^M (t-\tau),$$

$$X, Y, Z \in \Omega';\ \xi \geqslant 0;\ t \geqslant \tau \geqslant 0;\ X \neq Y,\ \text{si}\ t = \tau;\ \alpha, \beta = 1, ..., N.$$

N_1 est le nombre des différentes racines de l'équation de Petrovsky, pour $s^2 = 1$, μ_ν — l'ordre de la racine λ'_ν, $\nu = 1, ..., N_1$. Les coefficients $K_{\alpha\nu l}^\beta$, $l = 0, 1, ..., \mu_\nu$ de la somme (4',1) et les racines λ'_ν dépendent des coefficients de la matrice des quasi-solutions; ils sont donc les fonctions de (Z, ξ). Les fonctions v_α^β forment la matrice-solution $[v]$ du système auxiliaire bien connu des équations linéaires aux derivées entières, avec les valeurs initiales données par le symbole de Kronecker δ_α^β.

Il résulte de l'hypothèse I qu'on a uniformément pour $Z \in \Omega'$:

$$(5.1)\qquad \lim_{\xi\to\infty} \lambda'_\nu = \hat{\lambda}'_\nu, s^2 = 1; \lim_{\xi\to\infty} K_{\alpha\nu l}^\beta = \hat{K}_{\alpha\nu l}^\beta, l = 0, ... \mu_\nu, \nu = 1, ... N_1.$$

Alors les quasi-solutions du système (3.1) prendront la forme que voici:

$$(6.1)\qquad \hat{W}_{\alpha\beta}^Z = \hat{W}_{\alpha\beta}^Z(X, Y, \theta) = (2\pi)^{-n}\int_{-\infty}^{+\infty} \hat{v}_\alpha^\beta(\theta, Z; (s)) \exp i(s\cdot(x-y))\,dS,\ \theta = t-\tau$$

et

$$(6'.1)\qquad \hat{v}_\alpha^\beta = \hat{v}_\alpha^\beta(\theta, Z; (s)) = \sum_{\nu=1}^{N_1}(\hat{K}_{\alpha\nu l}^\beta \cdot s^{Ml}\theta^l)_{l=0}^{\mu_\nu} \exp \hat{\lambda}'_\nu s^M \theta, \qquad \alpha, \beta = 1, ..., N.$$

Les matrices $[\hat{v}]$ et $[\hat{W}\theta^{n/M}]$ sont composées de fonctions entières en $s\theta^{1/M}$ et $(X-Y)/\theta^{1/M}$ de classes Z_P^P et Z_q^q respectivement, avec $p = M$ et $1/p + 1/q = 1$, [5], [9].

Posons pour la matrice des solutions fondamentales, [5], du système (1,1):

$$(7.1)\qquad \Gamma_{\alpha\beta} = W_{\alpha\beta}^{Y,\tau} + \overline{W}_{\alpha\beta}, \alpha, \beta = 1, ..., N,$$

où le dernier composant est le potentiel bien connu de charge spatiale [5].

Plus précisément, la matrice des solutions fondamentales du système (3,1) sera:

$$(8,1)\qquad \hat{\Gamma}_{\alpha\beta} = \hat{W}_{\alpha\beta}^Y + \int_0^\theta \int_{\Omega'} \hat{S}(\hat{W}^\pi, \hat{\Phi})\,d\pi\,d\xi, \alpha, \beta = 1, ..., N, \quad \theta = t-\tau$$

où:

$$(8',1)\qquad \hat{S}(\hat{W}^\pi \hat{\Phi}) = \sum_{\gamma=1}^{N} \hat{W}_{\alpha\gamma}^\pi(X, \pi, \xi)\,\hat{\Phi}_{\gamma\beta}(\pi, Y, \theta-\xi).$$

$[\hat{\Phi}]$ est la solution d'un système d'équations intégrales, [5]; la matrice des noyaux de ce système est la suivante:

$$\hat{N}_{\alpha\beta} = \hat{N}_{\alpha\beta}(X, Y, \theta) = \hat{\hat{\psi}}^{(\alpha)}[\hat{W}^{Y}_{\alpha\beta}(X, Y, \theta)], \alpha, \beta \overset{\theta=t-\tau}{=} 1, \ldots, N. \tag{9,1}$$

En faisant intervenir la matrice des noyaux résolvants $[\hat{\mathfrak{R}}]$, on trouve pour la matrice $[\hat{\Phi}]$ les expressions:

$$\hat{\Phi}_{\alpha\beta} = \hat{N}_{\alpha\beta} + \int_0^{\theta} \int_{\Omega'} \hat{S}(\hat{\mathfrak{R}}, \hat{N})\, d\Pi\, d\xi, \alpha, \beta \overset{\theta=t-\tau}{=} 1, \ldots, N. \tag{9',1}$$

2. Supposons maintenant $n > M$. Nous allons intégrer les expressions (6,1) et (9,1) par rapport à θ, $0 \leqslant \theta \leqslant \infty$ en admettant:

$$\int_0^{\infty} \hat{W}^{Z}_{\alpha\beta}(X, Y, \theta)\, d\theta = w^{Z}_{\alpha\beta}(X, Y), \{w^{Z}_{\alpha\beta}(X, Y)\}_{\alpha,\beta=1,\ldots N} = [w^{Z}(X, Y)] = [w^{Z}], \tag{1,2}$$

et

$$\int_0^{\infty} \hat{N}_{\alpha\beta}(X, Y, \theta)\, d\theta = n_{\alpha\beta}(X, Y) = n^{0}_{\alpha\beta}(X, Y); \{n_{\alpha\beta}\}_{\alpha,\beta=1,\ldots N} = [n]; X \neq Y. \tag{2,2}$$

Faisons intervenir les noyaux itérés, leurs série infinie et la solution $\{\varphi_{\alpha\beta}\}_{\alpha,\beta=1,\ldots,N} = [\varphi]$.

$$n^{(\nu+1)}_{\alpha\beta}(X, Y) = \int_{\Omega'} s(n^{(0)}, n^{(\nu)})\, d\Pi; \tag{3,2}$$

$$\mathfrak{m}_{\alpha\beta}(X, Y) = \sum_{\nu=0}^{\infty} n^{(\nu)}_{\alpha\beta}(X, Y); \tag{4,2}$$

$$\varphi_{\alpha\beta}(X, Y) = n_{\alpha\beta}(X, Y) + \int_{\Omega'} s(\mathfrak{m}, n)\, d\tau; [\mathfrak{m}] = \{\mathfrak{m}_{\alpha\beta}\}_{\alpha,\beta=1,\ldots N}, \tag{5,2}$$

où:

$$s(n^{(0)}, n^{(\nu)}) = \sum_{j=1}^{N} n^{(0)}_{\alpha j}(X, Y, \Pi)\, n^{(\nu)}_{j\beta}(\Pi, Y) \text{ et } s, \mathfrak{m}, (n) \quad \sum_{j=1}^{N} \mathfrak{m}_{\alpha j}(X, \Pi)\, n_{j\beta}(\Pi, Y).$$

3. Soit la matrice des dominantes des fonctions (9,1):

$$\dot{N}_{\alpha\beta}(X, Y, \theta) = C[Nn^{M} C_0 (|XY|^{h} + \theta^{h'})\, \theta^{-1-n/M} + \sum_{1 \leqslant j \leqslant N}^{0 \leqslant m < M} a^{(\varkappa)}_{\alpha j}(X)\, \theta^{-(n+m)/M}] \exp[-c(|XY|/\theta^{1/M})^{q}], \tag{3,1}$$

où la constante C dépend des coefficients du système (1,1), $q = M/(M-1)$ et

$$a^{(\varkappa)}_{\alpha j}(X) = \operatorname*{Max}_{t \geqslant 0} |A^{(\varkappa)}_{\alpha j}(X, t)|;$$

les constantes C_0, h et h' sont originaires de la formule (2,1).

L'Hypothèse III. On admet le domaine d'intégration, Ω', et les coefficients du système (1,1) assujetis aux inégalités suivantes:

$$(2,3)\qquad \begin{cases} \int\limits_0^\theta \int\limits_{\Omega'} \sum\limits_{\beta=1}^N \dot{N}_{\alpha\beta}(X, Y, \xi)\, dY\, d\xi \leqslant b < 1\,; \\ \int\limits_0^\theta \int\limits_{\Omega'} \sum\limits_{\beta=1}^N \dot{N}_{\beta\alpha}(X, Y, \xi)\, dX\, d\xi \leqslant b\,; \alpha = 1, \ldots, N \end{cases}$$

pour toutes les valeurs $\theta \geqslant 0$ et $X \in \Omega$, $Y \in \Omega'$.

Lemme (1.3). *Les hypothèses* I—III *étant admises, la série* (4.2) *converge pour* $X \neq Y$, $X \in \Omega$, $Y \in \Omega'$.

Soit:

$$(3,3)\qquad \Gamma_{\alpha\beta}(X, Y) = w^Y_{\alpha\beta}(X, Y) + \int\limits_{\Omega'} s\,(w^\pi, \varphi)\, d\Pi,\ \alpha, \beta = 1, \ldots, N,\ X \neq Y,\ X \in \Omega\,.$$

Les hypothèses et les définitions ci-dessus permettent de démontrer le:

Théorème (1.3). *Les hypothèses* I—III *étant admises et* $M < n$, *les expressions* (3,3) *existent, sont intégrables par rapport à* $Y \in \Omega'$; *elles forment par rapport à* X *la matrice des solutions du système élliptique limite des équations*:

$$(4,3)\qquad \psi^{(\alpha)}(u) = \sum_{1 \leqslant j \leqslant N}^{0 \leqslant m \leqslant M} \hat{A}^{(x)}_{\alpha j}(X)\, D^m(u_j) \equiv 0\,,\ \alpha = 1, \ldots, N\,;\ X \in \Omega\,.$$

4. Hypothèse IV. Admettons le domaine Ω borné par la surface S et la fonction $\{\varrho_\alpha(X, t)\}_{\alpha=1, \ldots, N}$ définie, continue, bornée et intégrable sur la surface S pour chaque valeur du temps t. On a uniformément sur S:

$$(1,4)\qquad \lim_{t \to \infty} \varrho_\alpha(X, t) = \hat{\varrho}_\alpha(X),\ X \in S;\ \alpha = 1, \ldots, N.$$

Soient maintenant les potentiels de simple couche du système (1,1)

$$U_\alpha(X, t) = \int\limits_0^t \int\limits_S \sum\limits_{\beta=1}^N \Gamma_{\alpha\beta}(X, t; Q, \tau)\, \varrho_\beta(Q, \tau)\, dQ\, d\tau,\ \alpha = 1, \ldots, N,\ X \in \Omega$$

et du système (4,3)

$$(3,4)\qquad u_\alpha(X) = \int\limits_S \sum\limits_{\beta=1}^N \Gamma_{\alpha\beta}(X, Q)\, \hat{\varrho}_\beta(Q)\, dQ\,,\ \alpha = 1, \ldots, N,\ X \in \Omega\,.$$

En généralisant les thèses de la communication [1] il est aisé de démontrer le

Théorème (1,4). *Les hypothèses* I—IV *étant admises on a* $\lim\limits_{t \to \infty} U_\alpha(X, t) = u_\alpha(X)$, $X \in \Omega$, $\alpha = 1, \ldots, N$.

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MATHEMATICS

Solution of the Problem of Existence of Simple Radical Ring

by

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Presented by A. MOSTOWSKI on February 25, 1961

The purpose of this note is to announce the following

THEOREM. *There exists a simple ring with non-zero multiplication radical in the sense of Jacobson.*

The idea of the proof is the following. Let S^* be the algebra of all formal series $\varepsilon_0+\varepsilon_1 x+\varepsilon_2 y+\varepsilon_{11} x^2+\varepsilon_{12} xy+\varepsilon_{21} yx+ \ldots$ in two not commuting indeterminants x, y over the prime field Φ of characteristic 2. It is easy to see that an element $\varepsilon_0+\varepsilon_1 x+ \ldots \in S^*$ is a unit if and only if $\varepsilon_0 = 1$. Let S be the set of all non-units of S^*. The set S forms obviously and ideal in S^* and, since S^* is a ring with identity, (see [2] p. 21) S is a radical ring. It can be proved that the element x does not belong to the principal ideal $(x+yx^2y)_s \subset S$. Now let M_x be a maximal ideal containing the principal ideal $(x+yx^2y)_s$ to which the element x does not belong, and let J be a minimal non-zero ideal in the factor ring S/M_x. The elements $x = x+M_x$, $\bar{x}\,\bar{y} = xy+M_x$ and $\bar{x}\,\bar{y} = xy+M_x$ belong to J and since $x+(yx)(xy) \in M_x$ then $\bar{x} = (y\bar{x}\,\bar{y})(\bar{x}\,\bar{y})$. Therefore $J^2 \neq (\bar{0})$. Because J is a minimal ideal we have $J = J^2$ and by a lemma of Andrunakiïevitch ([1] p. 186) J is a simple ring. J as an ideal of homomorphic image of radical ring S is itself a radical ring. This ends the proof of our theorem.

The detailed proof of the announced theorem will be published in Fundamenta Mathematicae.

This result was presented at the meeting of Moscow Mathematical Society on December 20, 1960.

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MATHEMATICS

A Topological Characterization of Open Theories

by

R. SIKORSKI

Presented by E. MARCZEWSKI on February 25, 1961

Let $\mathcal{S}$ be a two-valued first-order predicate calculus such that the set of all free individual variables and the set of all terms are equipollent.

For every formalized theory $\mathcal{T}$ based on $\mathcal{S}$, the symbol $L(\mathcal{T})$ will denote the Lindenbaum algebra of the theory $\mathcal{T}$, i.e. the Boolean algebra obtained from the set F of all formulas in $\mathcal{T}$ by identification of formulas α, β if and only if both the implications $\alpha \rightarrow \beta$ and $\beta \rightarrow \alpha$ are theorems in $\mathcal{T}$. For every formula $\alpha \in F$, the the symbol $|\alpha|_{\mathcal{T}}$ will denote the corresponding element in $L(\mathcal{T})$. Let $\mathcal{L}(\mathcal{T})$ denote the set of all prime filters $\mathfrak{f}$ in $L(\mathcal{T})$ such that, for every formula $\alpha(x)$, if $|\bigcup_x \alpha(x)|_{\mathcal{T}} \in \mathfrak{f}$ then there exists a term τ such that $|\alpha(\tau)|_{\mathcal{T}} \in \mathfrak{f}$. For every formula $\alpha \in F$, let

$$\|\alpha\|_{\mathcal{T}} = \{\mathfrak{f} \in \mathcal{L}(\mathcal{T}) \colon |\alpha|_{\mathcal{T}} \in \mathfrak{f}\}.$$

Let

$$\boldsymbol{L}(\mathcal{T}) = \{\|\alpha\|_{\mathcal{T}} \colon \alpha \in F\}$$

and

$$\boldsymbol{L}_0(\mathcal{T}) = \{\|\alpha\|_{\mathcal{T}} \colon \alpha \in F \text{ is an open formula}\}.$$

$\boldsymbol{L}(\mathcal{T})$ is a Boolean algebra of subsets of $\mathcal{L}(\mathcal{T})$, and the mapping

$$H_{\mathcal{T}}(|\alpha|) = \|\alpha\|_{\mathcal{T}}$$

is a Boolean homomorphism from $L(\mathcal{T})$ onto $\boldsymbol{L}(\mathcal{T})$.

The set $\mathcal{L}(\mathcal{T})$ will be considered as a topological space, the class $\boldsymbol{L}_0(\mathcal{T})$ being assumed as the basis determining the topology in $\mathcal{L}(\mathcal{T})$. The space $\mathcal{L}(\mathcal{T})$ is totally disconnected.

THEOREM 1. *A theory $\mathcal{T}$ is open if and only if $H_{\mathcal{T}}$ is an isomorphism and the space $\mathcal{L}(\mathcal{T})$ is compact.*

In the case where $\mathcal{T} = \mathcal{S}$, we shall write simply $\mathcal{L}$ and $|\alpha|$ instead of $\mathcal{L}(\mathcal{S})$ and $\|\alpha\|_{\mathcal{S}}$ respectively.

For every formalized theory $\mathcal{T}$ based on $\mathcal{S}$, the symbol $\mathcal{K}(\mathcal{T})$ will denote the intersection of all the sets $\|\alpha\|$, where α is a theorem in $\mathcal{T}$.

THEOREM 2. *A theory $\mathcal{T}$ is open if and only if $\mathcal{K}(\mathcal{T})$ is closed in the topological space $\mathfrak{L}$ and, for every formula $\alpha \in F$, $\mathcal{K}(\mathcal{T}) \subset \|\alpha\|$ implies that α is a theorem in $\mathcal{T}$.*

Proofs of Theorems I and II will be published in my paper *On open theories*, to appear in one of the Polish mathematical journals.

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MATHEMATICS

Concerning Tchebyshev's Generalized Method of Solving Non-linear Functional Equations

by

M. ALTMAN

Presented by W. ORLICZ on February 28, 1961

In [2] we presented an approximate method of solving non-linear functional equations in Banach spaces. This method is actually an iterative method of the third order and may be regarded as an abstract analogue of the Tchebyshev's well-known method for finding the roots of a function. The abstract formalism of this method for operator equations in Banach spaces has been investigated by Nečepurenko [7] and Mertvetzova [5].

However, our generalization is essentially different from that in [5] and concerns the zero-elements of a non-linear functional in Banach spaces. In many cases we can reduce the problem of solving an operator equation to that of solving a functional equation in the sense of finding the zero-elements of a non-linear functional in Banach space. Moreover, the difficulties of applying the operator variant of Tchebyshev's method in practice are very great. Even in the case of Newton-Kantorovitch method we have such hypotheses like the existence of the inverse of the Fréchet derivative and the estimate of its norm. In addition, exploiting Kantorovitch's method we have to solve a linear operator equation at each iteration step. The difficulties of the same nature are much harder in the case of the operator variant of Tchebyshev's method. All these difficulties are obviated in our method investigated here. The main tool exploited in our investigation is the application of the majorant principle. This principle has been used by Kantorovitch [4] in order to examine the abstract Newton method. An application of the same principle to investigate our generalization of Newton's method is given in [3]. Further, Mirakov [6] examined the operator variant of Tchebyshev's method by using the majorant principle as well. In examination of our abstract variant of Tchebyshev's method we shall use here the same argument as in [1] where we investigated the abstract method of tangent hyperbolas for finding the zero-elements of a non-linear functional in Banach space.

Let X be a Banach space and let $F(x)$, $x \in X$, be a non-linear continuous functional defined on the closed sphere $S(x_0, r)$ in X with centre x_0 and radius r.

Consider the non-linear functional equation

$$F(x) = 0. \tag{1}$$

Let us assume that $F(x)$ is differentiable in the sense of Fréchet in the sphere $S(x_0, r)$; we denote by $F'(x)$, $F''(x)$ and $F'''(x)$ the first, second and third derivatives of $F(x)$, respectively.

For the sequence of linear functionals $F'(x_n)$, $x_n \in S(x_0, r)$ we choose a sequence of elements y_n of X such that

$$\|y_n\| = 1, \quad F'(x_n)\, y_n = \|F'(x_n)\|, \qquad n = 0, 1, 2, \ldots$$

provided that such a choice is possible.

The iterative method for solving Eq. (1) is defined as follows [2].

Let x_0 be the given initial approximate solution of Eq. (1). Then we put

$$x_{n+1} = x_n - \left[1 + \frac{1}{2} \frac{F''(x_n)\, y_n^2\, F(x_n)}{\|F'(x_n)\|^2}\right] \frac{F(x_n)}{\|F'(x_n)\|}\, y_n. \tag{2}$$

Sufficient conditions for the convergence of this process which assure also the existence of a solution of Eq. (1) are given in [2].

We shall now apply the majorant principle to investigate the method defined by formula (2).

For this purpose we consider the real equation

$$Q(x) = 0, \tag{3}$$

where $Q(x)$ is a real function of the real variable x, being three times continuously differentiable in the interval (z_0, z').

Following [4], [3] let us say that Eq. (1) possesses a real majorant equation [3], if the following conditions are fulfilled:

1° $\quad |F(x_0)| \leqslant Q(x_0), \quad z_0 \geqslant 0;$

2° $\quad \dfrac{1}{\|F'(x_0)\|} \leqslant B_0;$

where $B_0 = -\dfrac{1}{Q'(z_0)} > 0;$

3° $\quad \|F''(x)\| \leqslant Q''(z)$ if $\|x - x_0\| \leqslant z - z_0 \leqslant z' - z_0;$

4° $\quad \|F'''(x)\| \leqslant Q'''(z)$ if $\|x - x_0\| \leqslant z - z_0 \leqslant z' - z_0.$

Let us now construct the sequence of the approximate solutions z_n of Eq. (3) by the iterative method of Tchebyshev:

$$z_{n+1} = z_n - \left[1 + \frac{Q''(z_n)\, Q(z_n)}{[Q'(z_n)]^2}\right] \frac{Q(z_n)}{Q'(z_n)}, \qquad n = 0, 1, 2, \ldots \tag{4}$$

The following theorem contains sufficient conditions for the convergence of the process defined by formula (2). These conditions assure also the existence of a solution of Eq. (1).

THEOREM. *Let us assume that* Eq. (1) *possesses a majorant* Eq. (3) *such that*

1) $$[Q'(z_0)]^2 - 2Q''(z_0)\,Q(z_0) > 0,$$

2) Eq. (3) *has a positive solution and*

$$Q'(z) < 0 \quad \text{for} \quad z_0 \leqslant z \leqslant \frac{5}{4}z^*,$$

where z^* *is the smallest positive root of* Eq. (3).

Under these assumptions we assert that the process in (4) *converges to the solution* z^* *of* Eq. (3). Eq. (1) *has a solution* x^* *and the sequence of approximate solutions* x_n *defined by formula* (2) *converges to it. The error estimate is given by the following formula*

(5) $$\|x^* - x_n\| \leqslant z^* - z_n.$$

Proof. The proof of this Theorem makes use of a lemma contained in paper [1]. First of all, we shall show that the sequence of z_n is convergent. It follows from the hypotheses of the Theorem that this sequence is increasing. Thus, it is sufficient to prove that this sequence is bounded. In virtue of the lemma mentioned above by using a simple argument one can see that

$$z_n \leqslant \frac{5}{4}z^*, \qquad n = 0, 1, 2, \ldots,$$

where z^* is the smallest positive root of Eq. (3), greater than z_0. Using the same lemma again we infer that the sequence of

$$\frac{Q(z_n)}{Q'(z_n)} \to 0, \quad \text{as} \quad n \to \infty.$$

Hence, it follows from the conditions of the Theorem that

$$Q(z_n) \to 0, \text{ as } n \to \infty.$$

One can prove that

$$z_n \to z^*, \text{ as } n \to \infty.$$

We shall show that condition (5) is fulfilled. It is easy to see from the conditions of the Theorem that

(6) $$\|x_1 - x_0\| \leqslant z_1 - z_0.$$

We shall now show that all conditions 1°—4° are satisfied if element x_0 is replaced by element x_1. Using the analogue of Taylor's formula in the integral form we get

$$F(x_1) = \frac{1}{2}\,\frac{F^3(x_0)\,[F''(x_0)\,y_0^2]^2}{\|F'(x_0)\|^4} + \frac{1}{8}\,\frac{F^4(x_0)[F''(x_0)\,y_0^2]^3}{\|F'(x_0)\|^6} + \\ + \frac{1}{6}\int_{x_0}^{x_1} F'''(\bar{x})\,(x_1 - \bar{x})^3\,d\bar{x}.$$

A similar formula is true for $Q(z_1)$. Hence, by comparison, we get

$$|F(x_1)| \leqslant Q(z_1).$$

Since $Q''(z) \geqslant 0$, the derivative $Q'(z)$ increases still preserving the minus sign at point z_1. We shall show that condition 2° is satisfied for $x = x_1$. We have

$$\|F'(x_1)\| \geqslant \|F'(x_0)\| \left(1 - \frac{\|F'(x_1) - F'(x_0)\|}{\|F'(x_0)\|}\right).$$

Using the abstract analogue of the fundamental formula of the integral calculus, we obtain, by 3° and (6).

$$\|F'(x_1)\| \geqslant \|F'(x_0)\| \left(1 - \frac{\left\|\int_{x_0}^{x_1} F''(x)\,dx\right\|}{\|F'(x_0)\|}\right) \geqslant \|F'(x_0)\| \left(1 - \frac{\int_{z_0}^{z_1} Q''(z)\,dz}{\|F'(x_0)\|}\right) \geqslant$$

$$\geqslant \|F'(x_0)\| \left(1 + \frac{Q'(z_1) - Q'(z_0)}{Q'(z_0)}\right) = \|F'(x_0)\| \frac{Q'(z_1)}{Q'(z_0)}.$$

Hence, we get

$$\frac{1}{\|F'(x_1)\|} \leqslant -\frac{1}{Q'(z_1)}.$$

It is easy to see that conditions 3° and 4° ave also satisfied for x_1. In fact, if

$$\|x - x_1\| \leqslant z - z_1 \leqslant z' - z_1,$$

then we have, by (6),

$$\|x_1 - x_0\| \leqslant \|x - x_1\| + \|x_1 - x_0\| \leqslant z - z_1 + z_1 - z_0 = z - z_0 \leqslant z' - z_0.$$

In the same way as above we get the inequality

$$\|x_2 - x_1\| \leqslant z_2 - z_1$$

corresponding to that in (6), where x_1 and z_1 play the role of x_0 and z_0, respectively.

Thus, by induction, we obtain

$$\|x_{n+p} - x_n\| \leqslant z_{n+p} - z_n \tag{7}$$

for any positive integers n and p.

Since the sequence of z_n converges to z^*, we conclude that there exists an element x^* of the sphere $S(x_0, r)$, $t = z' - z_0$, such that

$$x_n \to x^* \text{ as } n \to \infty.$$

It follows from (7) that condition (5) is satisfied. It remains to prove that x^* is a solution of Eq. (1).

In virtue of the lemma used before we obtain

$$\frac{F'(x_n)}{\|F(x_n)\|} \to 0 \quad \text{as} \quad n \to \infty.$$

Since the functional F is continuous and the sequence of $\|F'(x_n)\|$ is bounded we conclude that x^* is a solution of Eq. (1).

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MATHEMATICS

Extension and Stability of Certain Iterative Methods for Solving Non-linear Functional Equations in Banach Spaces

by

M. ALTMAN

Presented by W. ORLICZ on February 28, 1961

1. In [2] we gave an iterative method for solving non-linear functional equations, which is in principle a generalization of Newton's method, but differs essentially from that given by L. V. Kantorovitch [7], the latter being applicable only to non-linear operator equations in Banach spaces. A further generalization of our method is given in [4]. This is an abstract generalization of the well-known method of Tchebyshev. We should mention that our formalism is essentially different from the operator variant of Tchebyshev's method investigated by other authors.*) Another generalization of our abstract variant of Newton's method is given in [5]. This is a generalization of a class of iterative methods of the higher order based on the application of König's theorem. In the case of the second order iterative methods of this class we obtain again Newton's method. The third order iterative methods of this class coincide with the method of tangent hyperbolas**). We should mention again that our formalism is not an operator variant of these classical methods. All these methods concern the approximate solutions of non-linear functional equations.

$$F(x) = 0, \tag{1}$$

where F is a continuous non-linear functional defined on the Banach space X.

In many cases one can reduce operator equations to functional equations of the same kind as in (1). This fact seems to be very important for the practice, since the application of the operator variant of these methods presents very great difficulties. In fact, we need the existence of the inverse of the Fréchet derivative and the estimate of its norm. In addition, at each iteration step we must solve a linear operator equation. This is the case of Newton's abstract method and iterative methods of higher order are much harder to apply.

Let us assume that the functional $F(x)$ is differentiable in the sense of Fréchet. Denote by $F'(x)$ the first Fréchet derivative of $F(x)$. All these iterative methods

*) For references see [4].

**) For references see [5].

mentioned above and being applied to solve Eq. (1) need the following construction of a sequence of elements of the space X.

Let x_n be the approximate solution of Eq. (1). Then we choose an element y_n of X such that

$$\|y_n\| = 1, \; F'(x_n)\, y_n = \|F'(x_n)\|, \qquad n = 0, 1, 2, \ldots \tag{2}$$

provided that such a choice is possible. Thus, we see that these methods are applicable only in the case when the norm $\|F'(x_n)\|$ of the linear functional $F'(x_n)$ is reached on the unit sphere. This is possible in the Banach space with a weakly compact unit sphere, for instance, in Hilbert space, in L^p-space or, more generally, in reflexive Banach spaces. But this is not the case in general Banach spaces.

In [1] we considered a special case when the element y_n in (2) is so chosen that the value $F'(x_n)\, y_n$ is sufficiently near to the norm $\|F'(x_n)\|$.

In the present note we give an extension of all these iterative processes which makes it possible to apply these methods in general Banach spaces. Thus, it is not necessary for our methods to suppose that condition (2) is satisfied exactly.

On the other hand, the accuracy in numerical calculations is limited and we have always a truncation error. However, the possibility of choosing the elements y_n shows that the convergence of these processes can be preserved. Hence, it follows the stability of the convergence of these methods.

The argument used here is based on the application of the majorant principle (see [3], [5], [6]).

Let us begin with the extension of Newton's method. This method is defined as follows.

$$x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)\, y_n}\, y_n, \qquad n = 0, 1, 2, \ldots \tag{3}$$

Let us assume that the second Fréchet derivative $F''(x)$ of $F(x)$ exists and is continuous in the sphere $S(x_0, r)$ with centre x_0 and radius r.

Consider now the real equation

$$Q(z) = 0, \tag{4}$$

where $Q(z)$ is a real function of the real variable z, being twice continuously differentiable in the segment (z_0, z').

Following the argument of paper [3] let us say that Eq. (1) possesses a real majorant equation (4), if the following conditions are satisfied.

1° $\quad |F(x_0)| \leqslant Q(z_0)$;

2° $\quad \dfrac{1}{\|F'(x_0)\|} < B_0, \; B_0 = -\dfrac{1}{Q'(z_0)} > 0$;

3° $\quad \|F''(x)\| \leqslant Q''(z)$, if $\|x - x_0\| \leqslant z - z_0 \leqslant z' - z_0$.

Let us further define the sequence of approximate solutions z_n of Eq. (4) by Newton's classical process, i.e.

$$z_{n+1} = z_n - \frac{Q(z_n)}{Q'(z_n)}, \quad n = 0, 1, 2, \ldots \tag{5}$$

The convergence of the process determined by conditions (2) and (3) consists in the following choice of the elements y_n in (2):

$$\|y_n\| \leqslant 1 \text{ and } |Q'(z_n)| \leqslant |F'(x_n)\, y_n| \leqslant \|F'(x_n)\|, \tag{6}$$

where z_n is defined by (5). The possibility of such a choice will be shown below.

The following theorem is an extension of the corresponding theorem of [3] and gives sufficient conditions of convergence of the process determined by conditions (3) and (6). These conditions also guarantee the existence of a solution of Eq. (1).

THEOREM 1. *If* Eq. (1) *possesses a real majorant equation* (4) *and if* Eq. (4) *has a real root in the segment* (z_0, z'), *then* Eq. (1) *has a solution* x^* *in the sphere* $S(x_0, r)$ *where* $r = z' - z_0$, *and the sequence of approximate solutions* x_n *constructed by process* (3), (6) *converges to it. For the error estimate we have the following formula*

$$\|x^* - x_n\| \leqslant z^* - z_n, \tag{7}$$

where z^* *is the nearest to* z_0 *root of* Eq. (4).

Proof. The proof of this Theorem is only in some details different from that of the corresponding theorem in paper [3]. We shall show only the possibility of the choice of the elements y_n to satisfy condition (6).

We have

$$\|F'(x_1)\| \geqslant \|F'(x_0)\| \left(1 - \frac{\|F'(x_1) - F'(x_0)\|}{\|F'(x_0)\|}\right).$$

Using the abstract analogue of the fundamental formula of the integral calculus, we obtain by 2° and 3°

$$\|F'(x_1)\| \geqslant \|F'(x_0)\| \left(1 - \frac{\left\| \int_{x_0}^{K_1} F''(x)\, dx \right\|}{\|F'(x_0)\|}\right) \geqslant \|F'(x_0)\| \frac{Q'(z_1)}{Q'(x_0)} > Q'(z_1).$$

Since $Q''(z) \geqslant 0$, the derivative $Q'(z)$ increases, still preserving the minus sign at point z_1. Thus, we get

$$\frac{1}{\|F'(x_1)\|} < -\frac{1}{Q'(z_1)}, \tag{8}$$

whence it results that condition 2° is also satisfied for x_1. Moreover, inequality (8) shows the possibility of the choice of the elements y_n to satisfy condition (6).

Remark 1. If we put

$$\frac{1}{\|F'(x_0)\|} \leqslant B_0 \tag{9}$$

instead of 2°, then we can only choose the elements y_n, $\|y_n\| \leqslant 1$, as in (2); i.e. so that $F'(x_n)\, y_n = \|F'(x_n)\|$, but such a choice is not always possible as is mentioned above. Thus, the fact that we have an exact inequality in 2° is essential. All results of paper [3] remain true under condition (6) if we replace everywhere the corresponding inequalities (9) by 2°.

Remark 2. Let us observe that the speed of the convergence of process (3) depends on the choice of the elements y_n in (6). In fact, if $\bar{y}_n$, $\|\bar{y}_n\| = 1$, is so chosen that the value $|F'(x_n)\,\bar{y}_n|$ becomes nearer to $\|F'(x_n)\|$, then process (3) converges more rapidly, since

$$\|\bar{x}_{n+1} - x_n\| = \frac{|F(x_n)|}{|F'(x_n)\,\bar{y}_n|}\,\|\bar{y}_n\| \geqslant \frac{|F(x_n)|}{\|F'(x_n)\|} = \frac{|F(x_n)|}{|F'(x_n)\,y_n|}\,\|y_n\| = \|x_{n+1} - x_n\|,$$

where

$$\|y_n\| = 1 \text{ and } |F'(x_n)\,y_n| = \|F'(x_n)\|$$

and x_{n+1} is the approximate solution corresponding to $\bar{y}_n$. We can see here, as is mentioned above, that the possibility of such a choice of the elements y_n determined by (6) preserves the convergence of process (3). This fact shows the stability of the convergence of this process.

2. We shall now apply the argument of sec. **1** to extend the generalized method of tangent hyperbolas and to show the stability of its convergence.

As in sec. **1** we suppose that Eq. (1) possesses a real majorant Eq. (4) which satisfies the conditions 1°—3° and, in addition

4° $$\|F'''(x)\| \leqslant Q'''(z), \text{ if } \|x - x_0\| \leqslant z - z_0 \leqslant z' - z_0.$$

Further, we define the sequence of approximate solutions z_n of Eq. (4) by the method of tangent hyperbolas

$$z_{n+1} = z_n - \frac{1}{1 - \frac{1}{2}\,\frac{Q''(z_n)\,Q(z_n)}{[Q'(z_n)]^2}} \cdot \frac{Q(z_n)}{Q'(z_n)}, \qquad n = 0, 1, 2, \ldots \tag{10}$$

Then the extension of the generalized method of tangent hyperbolas for Eq. (1) is defined by the following formula

$$x_{n+1} = x_n - \frac{1}{1 - \frac{1}{2}\,\frac{F''(x_n)\,y^2 F(x_n)}{[F'(x_n)\,y_n]^2}}\,\frac{F(x_n)}{F'(x_n)\,y_n}\,y_n, \tag{11}$$

where the elements y_n are so chosen as to satisfy condition (6) in which the elements z_n should be replaced by those of (10).

In the same way as in sec. **1** we obtain the following

THEOREM 2. *Suppose that* Eq. (1) *has a real majorant* Eq. (4) *such that conditions* 1°—4° *are satisfied;*

Eq. (4) *has a positive root and*

$$Q'(z) < 0 \quad \textit{for} \quad 0 \leqslant z_0 \leqslant z \leqslant \frac{4}{3}\,z^*, \tag{12}$$

where z^* *is the smallest positive root of* Eq. (4). *Then process* (10) *defined for* $Q(z)$ *converges to* z^*, *and* Eq. (1) *has a solution* x^* *to which process* (11) *converges. The error estimate is given by the formula* (7), z_n *being defined by* (10).

Notice that Remarks 1 and 2 remain true also in this case.

3. We shall now apply the same argument to the generalized method of Tchebyshev [4]. As in sec. **2,** let us assume that Eq. (1) possesses a real majorant Eq. (4) satisfying conditions 1°—4°.

Let us now construct the sequence of approximate solutions z_n of Eq. (4) by the iterative method of Tchebyshev:

$$z_{n+1} = z_n - \left[1 + \frac{Q''(z_n)\,Q(z_n)}{[Q'(z_n)]^2}\right]\frac{Q(z_n)}{Q'(z_n)}, \qquad n = 0, 1, 2, \ldots \tag{13}$$

We can now extend the generalized method of Tchebyshev by the following formula

$$x_{n+1} = x_n - \left[1 + \frac{1}{2}\,\frac{F''(x_n)\,y_n^2\,F(x_n)}{[F'(x_n)\,y_n]^2}\right]\frac{F(x_n)}{F'(x_n)\,y_n}\,y_n\,, \tag{14}$$

where the elements y_n are so chosen as to satisfy condition (6) in which the elements z_n should be replaced by those of (14).

Using the same argument as in sec. **2,** we obtain the following

THEOREM 3. *Suppose that* Eq. (1) *has a real majorant* Eq. (4) *such that conditions* 1°—4° *are satisfied;*

Eq. (4) *has a positive root and*

$$Q'(z) < 0 \quad \textit{for} \quad 0 \leqslant z_0 \leqslant z \leqslant \frac{5}{4}\,z^*, \tag{15}$$

where z^* *is the smallest positive root of* Eq. (4). *Then process* (13) *converges to* z^*, *and* Eq. (1) *has a solution* x^* *to which process* (14) *converges. The error estimate is given by the formula* (7), z_n *being defined by* (13).

Let us observe that Remarks 1 and 2 remain true also in this case.

Remark 3. Conditions (12) and (15) can be replaced by the following

$$Q'(z_n) < 0, \qquad n = 0, 1, 2, \ldots$$

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Excited States of Acetylene

by
W. WOŹNICKI

Presented by A. JABŁOŃSKI on December 1, 1960

It is well known from experimental results [1], [2] that the symmetry of molecules in excited states can differ entirely from that in the normal state. Hitherto, attempts to provide a consistent account of the facts failed to proceed further than the qualitative stage [3]. It is the aim of the present investigation to approach the problem, as exemplified by the acetylene molecule, by means the ASMO method. The acetylene molecule was chosen because Ingold and King [4], [5] have ascertained from its absorption spectrum that, while being linear in the normal state (symmetry $D_{\infty h}$, Fig. 1a), the C_2H_2 molecule becomes bent in the first excited state, when the H atoms assume the *trans* configuration and $\angle$ CCH = 120° (symmetry C_{2h}, Fig. 1b).

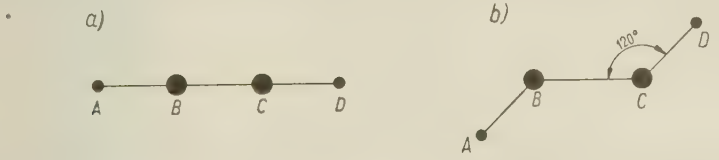

Fig. 1. The spatial configurations of the atoms in an acetylene molecule; B and C denote the carbon atoms, A and D — those of hydrogen; (a) normal state: r_{BC} 1.203 Å, r_{AB} r_{CD} 1.507 Å; (b) excited state: $r_{BC} = 1.383$ Å; $r_{AB} = r_{CD} = 1.08$ Å

Hitherto in dealing with the excited states of the acetylene molecule, only the π-electrons were considered [6], [7], whereas the remaining ones were summarily accounted for by introducing a suitable potential. However, in order to establish the correct relationship between the symmetry of the molecule and its energy state, all the valence electrons must necessarily be taken into account. Since employing an antisymmetric 10-electron wave function and the total Hamiltonian would represent a tedious procedure, the present investigation will start from the assumption that the electrons are divided into two classes: (1) the outer electrons, and (2) the inner ones constituting what is called the core.

The configuration of the normal state of the linear C_2H_2 molecule is the following:

$$\text{(I)} \qquad K^4(\sigma_g)^4_{CH}\,(\sigma_g)^2_{CC}\,(\pi_u)^4_{CC} \qquad \Sigma^+_g,$$

with K denoting the $1s$ shells, and the subsequent symbols — the molecular orbitals of the symmetry indicated, localized in the individual bonds. The symmetry species of the total wave function is indicated on the right hand side. If, on excitation, the molecule remains linear, the lowest configurations that can occur are:

$$\text{(II)} \qquad K^4 (\sigma_g)^4_{CH} (\sigma_g)^2_{CC} (\pi_u)^3_{CC} (\pi_g)^1_{CC} \qquad \Sigma_u^+, \Sigma_u^-, \Delta_u;$$

$$\text{(III)} \qquad K^4 (\sigma_g)^4_{CH} (\sigma_g)^2_{CC} (\pi_u)^3_{CC} (\sigma_u)^1_{CC} \qquad \Pi_g.$$

In either case, one of the electrons has been lifted from the bonding π_u orbital into the anti-bonding one π_g or σ_u, both having their respective charge-cloud concentrated, for the greater part, outside the C ≡ C region. Hence, quite considerable repulsion should be expected between the electron on each of these orbitals and the CH-bond electrons. Thus, the possibility suggests itself that, on excitation, the change in hybridization of the orbitals constituting the bonds will be such that the orbital receiving the excited electron shall be distributed as "far" as possible from the CH bond, i.e. the change in hybridization must occur in the direction from sp to sp^2. Change in hybridization involves a change in the angle CCH, so that the molecule assumes a bent form. The hydrogen atoms can now be situated in two ways, leading to either the *trans* or *cis* configuration. In view of the experimental data [4], only the former will be considered. As a result of the change in hybridization of the atomic orbitals in the plane of the molecule "disruptio" of one of bonding π_u orbitals will occur and in its place two lone atomic orbitals will arise. As a matter of fact, these orbitals must be expected to interact slightly, and form two molecular orbitals: a weakly bonding one ψ' of species b_u, and a weakly anti-bonding one ψ'' of species a_g. Hence, the electronic configurations of the bent molecule are the following: normal state

$$\text{(IV)} \qquad K^4 (\sigma_g')^4_{CH} (a_g)^2_{CC} (a_u)^2_{CC} (b_u \psi')^2_{CC} \qquad A_g;$$

as the CCH angle tends towards 180°, this configuration tends towards the linear one (I); lowest excited states

$$\text{(V)} \qquad K^4 (\sigma_g')^4_{CH} (a_g)^2_{CC} (a_u)^1_{CC} (b_u \psi')^2_{CC} (a_g \psi'')^1_{CC} \qquad A_u,$$

$$\text{(VI)} \qquad K^4 (\sigma_g')^4_{CH} (a_g)^2_{CC} (a_u)^1_{CC} (b_u \psi')^1_{CC} (a_g \psi'')^2_{CC} \qquad B_g;$$

as the molecule straightens, configuration (V) transforms into (III).

Ingold and King established that the band they had observed was related to an electronic transition polarized perpendicularly to the plane of the molecule. The allowed transition of such polarization is $\Sigma_g^- \rightarrow A_u$. Thus, in considering the energy as a function of the angle CCH, we shall restrict ourselves to configurations (IV) in the normal state and (V) in the lowest excited state.

In constructing the molecular orbitals, the two-centre approximation will be applied, i.e. they are constructed from the atomic orbitals of two neighbouring centres. The valence state of either of the carbon atoms in a bent acetylene molecule

is $(1s)^2\,(\varphi_1)^1\,(\varphi_2)^1\,(\varphi_3)^1\,(2p_z)^1$, with $\varphi_i\,(i = 1, 2, 3)$ denoting three atomic orbitals (hybrids) directed in three different directions in the plane of the molecule (Fig. 2), and $2p_z$ — the atomic orbital directed perpendicularly thereto. Quite generally,

$$\varphi_i = (1+\lambda_i^2)^{-1/2}\,(s + \lambda_i\, p_i), \tag{1}$$

where s denotes an orbital of type $2s$, p_i — one of type $2p$ directed in the i-direction, and λ_i the respective hybridization parameter. The molecular orbitals are of the form (Fig. 2)

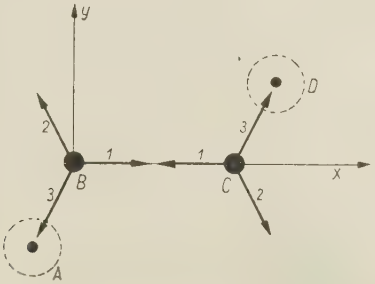

Fig. 2. Directions of the atomic orbitals φ_i, and their mutual relationship in space

$$(2)\quad \begin{cases} \psi_1 = N_1\,(k\varphi_{B3} + \varphi_A) & (\sigma_g')_{CH}, \quad \psi_4 = N_4\,(\varphi_{Bz} + \varphi_{Cz}) & (a_u)_{CC}, \\ \psi_2 = N_2\,(k\varphi_{C3} + \varphi_D) & (\sigma_g')_{CH}, \quad \psi_5 = N_5\,(\varphi_{B2} - \varphi_{C2}) & (b_u\,\psi')_{CC}, \\ \psi_3 = N_3\,(\varphi_{B1} + \varphi_{C1}) & (a_g)_{CC}, \quad \psi_6 = N_6\,(\varphi_{B2} + \varphi_{C2}) & (a_g\,\psi'')_{CC}. \end{cases}$$

The symbols on the right hand side denote the symmetry of the respective molecular orbitals, whilst φ_z stands for a function of type $2p_z$, and φ_A, φ_D are orbitals of type $1s$ of the hydrogen atom, k is a measure of the polarity of the CH bonding orbital, and $N_i\,(i = 1, \ldots, 6)$ are appropriate normalization constants. It is readily shown that ψ_4, ψ_5 and ψ_6 are mutually orthogonal, and that as the molecule straightens they transform into bonding and anti-bonding orbitals of π-type. It is precisely for this reason that the aforementioned classification of the electrons is carried out in such a manner that those occupying the ψ_4, ψ_5 and ψ_6 orbitals are considered to be outer electrons, whereas the remaining ones constitute the core. The assumption is made that the angle CCH is equal to the angle θ_{13} between the atomic orbitals φ_1 and φ_3. The relationship between this angle and the hybridization parameters can be established from the conditions of orthogonality of the atomic orbitals φ_i [8], [9]. This yields

$$\cos\theta_{ij} = -(\lambda_i\,\lambda_j)^{-1}, \quad (i, j = 1, 2, 3). \tag{3}$$

The parameters λ_i are not independent. From the condition $\theta_{12} + \theta_{13} + \theta_{23} = 2\pi$ we have

$$\lambda_1^2\cdot\lambda_2^2\cdot\lambda_3^2 + (\lambda_1^2 + \lambda_2^2 + \lambda_3^2) = 2. \tag{4}$$

The atomic orbitals forming part of the bonding orbitals $(\sigma'_g)_{CH}$ and $(a_g)_{CC}$ are assumed to possess equal parameters of hybridization, $\lambda_1 = \lambda_3 = \alpha$. In this case it yields

$$\Theta_{13} = \arccos\left(-\frac{1}{\alpha^2}\right). \tag{5}$$

The quantity k^2, which provides a measure of the distribution of the charge related to a given orbital between the C and H atoms, is assumed, after W. Kołos [9], to be equal to the ratio of the electronegativity of these atoms [10]. With this assumption, $k = 1.09$. It should be stressed that, for this value of k, the integrals $\int \psi_m^* \psi_n \, d\tau$ $(m, n = 1, 2, 3)$ are of the order of 0.01, so it may be accepted that the ψ_1, ψ_2 and ψ_3 orbitals occupied by the electrons of the core are approximately orthogonal.

In computing the total energy of the molecule, the ASMO method is applied, [11], [12]. By (IV), (V) and (2), the antisymmetric wave function of the outer electrons has the form

$$\Psi_0\,(^1A_g) = \|\psi_4\,\bar{\psi}_4\,\psi_5\,\bar{\psi}_5\|, \tag{6}$$

*)

$$\Psi_0(^1A_u) = 2^{-1/2}(\|\psi_4\,\psi_5\,\bar{\psi}_5\,\bar{\psi}_6\| - \|\bar{\psi}_4\,\psi_5\,\bar{\psi}_5\,\psi_6\|), \tag{7}$$

where e.g.,

$$\|\psi_4\,\psi_5\,\psi_5\,\psi_6\| = (4!)^{-1/2} \det\{\psi_4(1)\,\alpha(1) \quad \psi_5(2)\,\alpha(2) \quad \psi_5(3)\,\beta(3) \quad \psi_6(4)\,\beta(4)\}.$$

For either state ^1A_g and ^1A_u, the electrons of the core are described by the same function

$$\Psi_c = \|\psi_1\,\bar{\psi}_1\,\psi_2\,\bar{\psi}_2\,\psi_3\,\bar{\psi}_3\|. \tag{8}$$

The total energy is

$$E = E_n + E_o + E_c + E_{co}^{\text{int}}, \tag{9}$$

where E_n denotes the energy of Coulomb interaction of the nuclei, E_o — the energy of the outer electrons, E_c — that of the electrons of the core, and E_{co}^{int} — that of the interaction between the outer electrons and the core. From Fig. 1b it is seen that

$$E_n = \frac{Z^2}{r_{BC}} + \frac{Z}{r_{AC}} + \frac{Z}{r_{BD}} + \frac{Z}{r_{AB}} + \frac{Z}{r_{CD}} + \frac{1}{r_{AD}}, \tag{10}$$

$Z = 4$ being the effective charge of a C nucleus (the $1s$ electrons are assumed to be entirely swallowed up by the nucleus). The energy of the outer electrons is

$$E_o = E_o^{\text{orb}} + E_o^{\text{int}}, \tag{11}$$

where E_o^{orb} is the sum of the energies of the electrons on the occupied orbitals:

$$E_o^{\text{orb}}(^1A_g) = 2\varepsilon_4 + 2\varepsilon_5, \qquad E_o^{\text{orb}}(^1A_u) = \varepsilon_4 + 2\varepsilon_5 + \varepsilon_6, \tag{12}$$

*) Only sinlet states are considered.

with

$$\varepsilon_\mu = \int \psi_\mu^*(\vec{r}) \left[-\frac{1}{2} \Delta + \sum_\alpha \frac{Z_\alpha}{r_{\alpha\mu}} \right] \psi_\mu(\vec{r})\, d\tau. \tag{13}$$

In the last expression, the index α numbers the various nuclei in the molecule, and Z_α is their effective charge. E_o^{int} is the energy of interaction of the outer electrons:

$$E_o^{\text{int}} = \int \cdots \int \Psi_o^* \sum_{i>j} \frac{1}{r_{ij}} \Psi_o\, d\tau_1 \ldots d\tau_4 . \tag{14}$$

On substituting (6) or (7) into this expression, we have

$$\begin{cases} E_o^{\text{int}}(^1A_g) = \gamma_{55} + \gamma_{44} + 4\gamma_{54} - 2\delta_{54}, \\ E_o^{\text{int}}(^1A_u) = \gamma_{55} + 2\gamma_{54} + 2\gamma_{56} + \gamma_{46} - \delta_{54} - \delta_{56} + \delta_{46}, \end{cases} \tag{15}$$

with

$$\gamma_{kl} = \int\int \psi_k^*(\vec{r}_1)\, \psi_l^*(\vec{r}_2) \frac{1}{r_{12}} \psi_k(\vec{r}_1)\, \psi_l(\vec{r}_2)\, d\tau_1\, d\tau_2, \tag{16}$$

$$\delta_{kl} = \int\int \psi_k^*(\vec{r}_1)\, \psi_l^*(\vec{r}_2) \frac{1}{r_{12}} \psi_l(\vec{r}_1)\, \psi_k(\vec{r}_2)\, d\tau_1\, d\tau_2. \tag{17}$$

The energy of the electrons of the core, E_c, is computed likewise.

By analogy with (11), (12) and (15), we have now

$$E_c = E_c^{\text{orb}} + E_c^{\text{int}}, \tag{18}$$

$$E_c^{\text{orb}} = 2\varepsilon_1 + 2\varepsilon_2 + 2\varepsilon_3, \tag{19}$$

$$E_c^{\text{int}} = 2\gamma_{11} + \gamma_{33} + 4\gamma_{12} + 8\gamma_{13} - 4\delta_{13} - 2\delta_{12}. \tag{20}$$

The energy of interaction between an electron on the μ-th outer orbital and the core is given by

$$\varepsilon_\mu^{\text{int}} = \sum_\nu \int\int \psi_1^*(\vec{r}_1)\, \psi_1^*(\vec{r}_2) \ldots \psi_3^*(\vec{r}_6)\, \psi_\mu^*(\vec{r}_i) \times \times \frac{1}{r_{\nu i}} (-1)^P \hat{P} [\psi_1(\vec{r}_1)\, \psi_1(\vec{r}_2) \ldots \psi_3(\vec{r}_6)\, \psi_\mu(\vec{r}_i)]\, d\tau_\nu\, d\tau_i, \tag{21}$$

where $\nu\,(= 1, \ldots, 6)$ is the index of the electrons of the core, i — that of the outer electrons, and $\hat{P}$ is the usual permutation operator for the electrons. Thus

$$E_{co}^{\text{int}} = \sum_\mu \varepsilon_\mu^{\text{int}} \tag{22}$$

the summation is extended over all the occupied outer orbitals. For the purpose of computing the quantity (21), it is assumed that the inner shell electrons occupy the atomic orbitals q_ν constituting ψ_1, ψ_2 and ψ_3. Now (21) can be represented

as the sum of the Coulomb and exchange interactions with each of the inner electrons (see, e.g., [13]):

$$\varepsilon_{\mu}^{\text{int}} = \sum_{\nu} \left[\int\int \varphi_{\nu}^{*}(\vec{r}_1)\, \psi_{\mu}^{*}(\vec{r}_2) \frac{1}{r_{12}} \varphi_{\nu}(\vec{r}_1)\, \psi_{\mu}(\vec{r}_2)\, d\tau_1\, d\tau_2 - \right.$$

$$\left. - \frac{1}{2} \int\int \varphi_{\nu}^{*}(\vec{r}_1)\, \psi_{\mu}^{*}(\vec{r}_2) \frac{1}{r_{12}} \psi_{\mu}(\vec{r}_1)\, \varphi_{\nu}(\vec{r}_2)\, d\tau_1\, d\tau_2 \right]. \tag{23}$$

In order to compute all the integrals, it is necessary to substitute ψ_i ($i = 1, \ldots, 6$) from (2) and, subsequently, φ_k from (1), into the expressions of the type (13), (16), (17), and (21). Functions of the Slater type are used for representing the C atom $2s$ and $2p$ orbitals, assuming a value of $\delta = 1.625$ [10]. Thus, the problem of calculating the integrals over molecular orbitals reduces to one of evaluating integrals over atomic orbitals. A number of these can be reduced to integrals tabulated by Kotani et al. [14], [15] and Preuss [16], whereas the remaining ones had to be computed. With respect to the three- and four-centre integrals this was done by applying the Mulliken approximation.

The Table shows the dependence of the total energy of the molecule, as well as of its component parts, on the parameter of hybridization and on the angle CCH. It is seen that the total energy E for the normal state ^1A_g attains its minimum value at $\theta_{13} = 180°$. This means that the normal state of the bent molecule is not stable, and we are induced to conclude that acetylene in the normal state is linear and possesses the symmetry $^1\Sigma_g^+$, as corroborated by the experimental data. Moreover, for the excited state ^1A_u, E is seen to assume its lowest value at $\theta_{13} = 120°$. Hence,

TABLE

Total energy of the molecule and that of its component parts, versus the parameter of hybridization α (versus angle Θ_{13}), in atomic units

α		1	1.2	1.3	$\sqrt{2}$	1.6	2
Θ_{13}		180°	134°	126°	120°	113°	104°
E_c^{orb}		—26.4832	—26.7238	—26.8000	—26.8618	—26.9273	—26.9478
E_c^{int}		5.4705	5.7218	5.8262	5.9469	6.0202	6.0718
E_c		—21.0127	—21.0020	—20.9738	—20.9149	—20.9071	—20.8760
E_n		11.9129	12.0711	12.1341	12.1956	12.2765	12.3954
E_o^{orb}	^1A_g	—16.2460	—16.2788	—16.3698	—16.4851	—16.4980	—16.4776
	^1A_u	—16.0000	—16.1241	—16.2641	—16.4381	—16.4757	—16.5368
E_o^{int}	^1A_g	2.7064	2.6515	2.6346	2.6201	2.6042	2.5868
	^1A_u	2.6221	2.5588	2.5403	2.5260	2.5132	2.5077
E_o	^1A_g	—13.5396	—13.6273	—13.7352	—13.8650	—13.8938	—13.8908
	^1A_u	—13.3779	—13.5653	—13.7238	—13.9121	—13.9625	—14.0291
E_{co}^{int}	^1A_g	9.3120	9.2673	9.3098	9.3650	9.3871	9.3986
	^1A_u	9.3161	9.1813	9.1841	9.2008	9.1825	9.1573
E	^1A_g	—13.3275	—13.2908	—13.2651	—13.2194	—13.1373	—12.9727
	^1A_u	—13.1617	—13.3150	—13.3793	—13.4306	—13.4106	—13.3523

it is to be concluded that, in the excited state, the molecule is bent and the angle CCH presents a value in accordance with the experimental data [4], [5]. The energy of the transition $^1\Sigma_g^+ \rightarrow {}^1A_u$ amounts to 6.38 eV, corresponding to a wave length of $\lambda \approx 1950$ Å of the absorbed light, which is quite reasonable with respect to the known experimental results. The data assembled in the Table give insight into the role played by the various component parts of the total energy of the molecule. It will be noted that the energy of the outer electrons E_o is decisive in determining the shape $E = f(\alpha)$ (strictly, it is the ε_6 component of the energy i.e. that of the electron occupying the $(a_g \psi'')_{CC}$ orbital). The least variable component is E_c; nevertheless, the correct shape of $E = f(\alpha)$ and results in accordance with experiment can only be obtained, if all the components in the energy are taken into account. Hence, the role of the π electrons and, in particular, that of the $\pi - \sigma$ type interaction is essential and cannot be neglected in molecular calculations. Moreover, the results of the present investigation would seem to speak in favour of the non-empirical ASMO method as being well adapted to the solution of problems relating to the structure of molecules in the excited state, within the limits of the present investigation.

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Electrical Properties of the CdTe-HgTe System

by

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Preparation of the materials composing the CdTe-HgTe system is described. The results obtained on the latter measuring the electric conductivity and the Hall coefficient in the temperature range of 190°K to 540°K are given. The greatest variations of the current carrier mobility occur when the composition of the system is made to vary in the region of high HgTe content.

From the discussion of the preparation and properties of semiconductor mixed crystals of type $A^{III}B^{V}$ and $A^{II}B^{VI}$ such as InAs-InP, InSb-GaSb, ZnTe-CdTe, etc. in [1]—[3], the lattice constant is seen to vary linearly with the composition of the solid solution. The width of the forbidden zone, as well as other parameters, are generally found to vary continuously.

It was felt that the CdTe-HgTe system [4], [5] should be of interest in this respect as both CdTe [6] and HgTe [7], [8] belong to the same crystal system and their lattice constants are very similar. On the other hand, the semiconducting properties of CdTe and HgTe differ strongly so that the two compounds should be expected to yield a semiconductor presenting the present values of the parameters within the interval determined by those of CdTe and HgTe.

	Crystal system	Lattice constant [Å]	ΔE [eV]	μ mobility [cm²/Vsec] (at 300°K)	effective mass m^* [m_0]	melting point [°C]
CdTe	zinc blende	6.4588	1.45	600	0.37	1100
HgTe	zinc blende	6.4400	0.02	25000	0.04	670

Preparation of CdTe-HgTe system

The elements Cd, Te and Hg of a high degree of purity (10^{-5}%) were used, obtained by means of distillation *in vacuo* and zone melting [9] starting from material of technical purity. Preparation of the CdTe-HgTe solution was carried out in two steps: first, the compound HgTe was prepared by melting, and then the quantities

of Cd and Te corresponding to a given amount of HgTe were added so that by melting these components together a solid HgTe-CdTe solution of known per cent composition was obtained. The components were weighed to within 10^{-5}%. The above described preparation was carried out in quartz tubes sealed off under vacuum (10^{-5} mm. Hg.) at a temperature exceeding the melting point of the system (by about 50° to 100°) during 5—6 hours with subsequent slow cooling. This yielded a material of the required quantitative composition.

The compound HgTe was obtained by heating the required amounts of Hg and Te at 360°C for 20 hours and then at 750°—800°C for 4 hours and cooling slowly.

In the process of preparation some samples were found to give off pure Hg in amounts of 2—3% of the total Hg content. In the case of $Cd_{0.6}Hg_{0.4}Te$ and samples of higher Cd content instead of Hg a brown, brittle excrescence easily detachable from the bulk of the material appeared. As the CdTe content in the solution increases, the material becomes more brittle and less easy to separate from the quartz. Well crystallized samples are more readily detached from the quartz.

Measurement of electrical conductivity and Hall coefficient

The electrical conductivity and Hall coefficient were measured in samples of higher HgTe content. The measurements were carried out at constant current and constant magnetic field strength; voltages were measured with a multi-point recording potentiometer. All values were measured at intervals of 6 seconds, so that the experimental curves can be considered to provide a continuous representation.

Fig. 1 shows the temperature dependence of the electrical conductivity for several samples. Fig. 2 shows the temperature dependence of the Hall coefficient, whereas Fig. 3 shows the product $R\sigma$ versus the temperature. The figures at the ends of the curves denote the molar per cent content of HgTe in the sample.

Bends appear in all curves (except 50) of the temperature dependence of the Hall coefficient and electrical conductivity. Bend points on the conductivity curves correspond approximately to those of the Hall coefficient curves.

The segment of the straight line between the bend points for sample 80 and the low temperature straight segment of the other samples can be interpreted as the result of excitation of carriers to the conductivity band from deep impurity levels (near the valence band) or from the full impurity band formed by these levels. These levels may be due primarily to deviations from stoichiometry (excess Te).

The steeper straight segment following the bend point corresponds to an intrinsic semiconductor. Towards higher CdTe contents the Hall coefficient increases and the conductivity decreases.

From Fig. 2 it is clearly seen that at higher temperatures, where impurities cease to play a role, the conductivity increases with the HgTe content. As the latter rises from 80% to 90%, the conductivity increases by one order of magnitude. The curves of Fig. 3 point to the existence of several distinct, competing mechanisms of scattering, which vary according to the quantitative make-up of the sample. The product

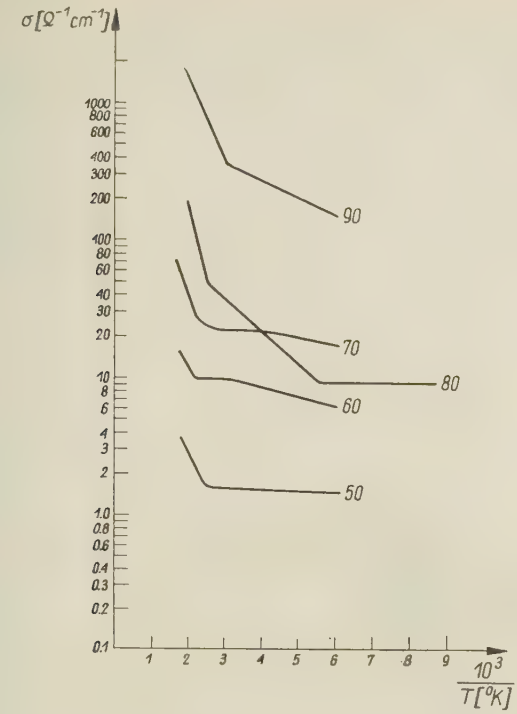

Fig. 1. Temperature dependence of electric conductivity σ

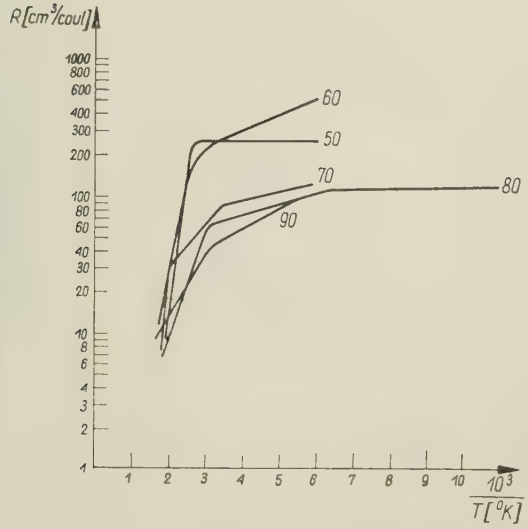

Fig. 2. Temperature dependence of Hall coefficient R

$R\sigma$ can be interpreted as the mobility, only when considering the low temperature segments of the curves corresponding to n-type impurity conductivity. An interpertation of the $R\sigma$-curves as the mobility throughout the entire temperature range would be justified only, if $\mu_n \gg \mu_p$, which does not seem to be the case.

The steepest changes of the product $R\sigma$ occur between 80% and 90% HgTe exactly as in the case of the conductivity.

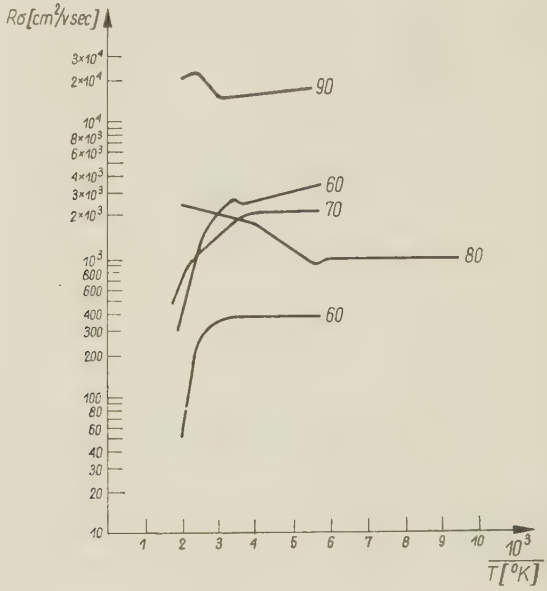

Fig. 3. Temperature dependence of product $R\sigma$

On the assumptions of a homogeneous and isotropic semi-conductor and of a predominant scattering process on acoustical phonons, the width ΔE of the forbidden gap can be calculated from the $\sigma = \sigma(T)$ or $R = R(T)$ curves. The dispersion of the values of ΔE thus obtained is considerable, ranging from 0.25 eV to 1.0 eV for the samples measured. Probably two factors contribute towards this: firstly, the assumptions underlying the formulas employed may not correspond to the true state of these semiconductor; secondly, the ΔE value is strongly affected by deviations from stoichiometry (Hg deficit). All samples changed their conductivity when illuminated.

The authors wish to thank Professor L. Sosnowski for his interest in the present investigation and for his valuable advice. They are indebted to J. Rałuszkiewicz for constructive discussion of the problem.

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On Relative Doublet Line Strengths in the Principal Series of Cesium

by
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Presented by W. RUBINOWICZ on January 13, 1961

It is well known that the doublet intensity ratios in the principal series of the spectra of alkalis are in general different from the value 2 (determined by the statistical weights ratio of the doublet levels). Theoretical arguments given by Fermi [3] explain this deviation by the spin-orbit interaction of the external electron. Similar effects, less systematically investigated, exist in many other spectra.*) Some aspects of this problem have as yet remained unexplained even for the best known case of the alkalis. So far, only a rough numerical estimation of the Fermi formula for a few initial members of the series has been given. The main cause is the insufficient knowledge of radial integrals involved in this formula (Their importance has been stressed by Sambursky [17]). This makes the computations for further lines of the series very uncertain, if not quite impossible, and does not allow an exact estimation of the true agreement between this formula and experimental data for them. It seems that new calculations for principal series of the spectra of alkalis taking into account as many radial integral values as possible, can throw some light on this problem (common to all one-electron spectra). Explicit computations are given for Cs, for which the spin-orbit interaction assumes the largest values, and the necessary number of radial integrals is known; moreover, the greatest controversy exists for this element between different experimental results. Their confrontation with theoretical assumptions seems therefore particularly interesting.

Formula of Fermi. Quantities necessary for its evaluation

It is given after Fermi [3] (in symbols introduced in [8]):

$$\left(\frac{S_2}{S_1}\right)_n = 2\left(\frac{1 + 1/3\, F_n}{1 + 2/3\, F_n}\right)^2, \tag{1}$$

where S_1, S_2 are line strengths of the doublet components with upper $^2P_{1\,2}$ and $^2P_{3/2}$ levels, respectively, and

*) An attempt to generalize the Fermi formula for principal, sharp and diffuse series of Al, Ga, In and Tl has been given by the author [8].

(2) $$F_n = \sum_{k \neq n} \frac{\sqrt{\Delta_{n1}\,\Delta_{k1}}}{E^0_{n1} - E^0_{k1}} \frac{\varrho_{10,k1}}{\varrho_{10,n1}},$$

(3) $$\Delta_{n1} = E_{n,1,3/2} - E_{h1,1/2},$$

(4) $$\varrho_{10,n1} = \int_0^\infty R^0_{10} R^0_{n1} r^3 \, dr,$$

where R^0_{nl} represents the unperturbed radial functions and n — the conventional quantum number ($n = 2, 3, \ldots$). As stressed by Fermi, the form of (1) allows, at least in principle, to express by the experimental data all quantities appearing in it. This is evident for Δ_{nl} and E^0_{nl}, but possible also for $\varrho_{10,n1}$. The latter can be expressed by the total line strengths of unresolved doublets. These strengths in turn are related in a simple way to the corresponding effective oscillator strengths; or in general

(5) $$S = \mathcal{S}(\mathcal{M})\,\mathcal{S}(\mathcal{L})\,\sigma^2$$

(6) $$\sigma^2 = \frac{1}{4l^2 - 1}\varrho^2,$$

where l denotes the greater of the two azimuthal quantum numbers of the transition (here $l = 1$), and $\mathcal{S}(\mathcal{M})$, $\mathcal{S}(\mathcal{L})$ are some factors (given by Goldberg [6], [7], White and Eliasen [21] or Russel [15]), depending on the transition; they are equal for all terms contributing to (2). Therefore, denoting two arbitrary integrals (4) by ϱ', ϱ'' we have

(7) $$\frac{\varrho'}{\varrho''} = \sqrt{\frac{s'}{s''}}.$$

On the other hand

(8) $$f_{k \to k'} = \frac{8\pi^2 mc}{3he^2} \frac{1}{g_k \lambda} S_{kk'},$$

with h, e, m, c, λ having their usual significance, k and k' denoting the set of quantum numbers for the lower and upper levels, respectively, and g_k being the statistical weight of the lower level. Combining (7) and (8) we obtain

(9) $$\frac{\varrho'}{\varrho''} = \sqrt{\frac{f'\lambda'}{f''\lambda''}} = \sqrt{\frac{f'\tilde{\nu}''}{f''\tilde{\nu}'}},$$

therefrom the ϱ-ratios can be computed when the corresponding f-values are known.

Obviously, besides this way of obtaining radial integrals, their theoretical values — when known — may be used. Both kinds of data were indeed used by Fermi. Theoretical values, calculated from the tables of Bates and Damgaard [1], were introduced by the present author [8] for the third column elements. However, the number of ϱ-values, possible to be obtained in this way is in general too small for our purpose as a gradually increasing number of terms must be retained in the sum (2), when n is increasing.

Numerical results

E^0_{nl} and Δ_{nl} have been calculated from spectroscopic data given by Kratz [10]; relative values of

$$f_n = \frac{f_{10\to n1}}{f_{10\to 21}} \tag{10}$$

and

$$\varrho_n = \frac{\varrho_{10\to n1}}{\varrho_{10\to 21}} \tag{11}$$

(given in Table I) result from experimental f-values of Minkowski, Mühlenbruch [11], Roschdestvensky, Füchtbauer and Waibel [20]. *) These are probably all experimental data for Cs (till 1959). **)

The known theoretical data, though too incomplete to be used, are also given for comparison in Table I. These are: one value of Gentile and Maiorana [5] used by Fermi, being in accord with the result of Minkowski and Mühlenbruch, and three ϱ-values resulting from the tables of Bates and Damgaard, the third being very uncertain. They are somewhat higher than those, obtained by other, theoretical or experimental, methods. (Some calculations of Mutô [12], mentioned by Korff and Breit [9] have been inaccessible to the author).

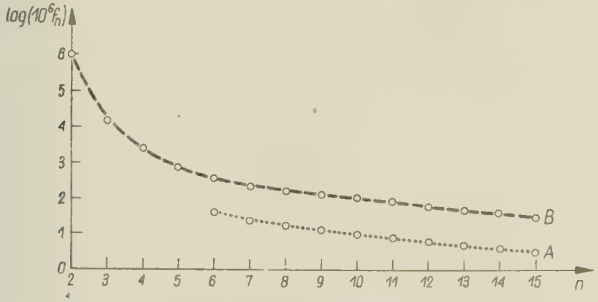

Fig. 1. Plot of log ($10^6 f_n$) against n

In order to verify the compatibility of experimental f-values of different origin, the plot of log ($10^6 f_n$) against n is given in Fig. 1 (the immaterial factor 10^6 has been introduced in order to omit negative values of the logarithms). Its inspection, shows that probably all f-values of Waibel [20] are too small, while their relative magnitudes seem to be measured with a good accuracy. This should not be deemed strange, as relative f-values are much easier to be established than absolute ones. One may even risk the assumption, that they are by one order lower than the correct

*) The results of Minkowski, Mühlenbruch as well as those of Waibel are quoted by Korff and Breit [9]. The older measurements of Roschdestvensky and Füchtbauer (performed in the years 1912—1926) are cited by Wolf and Herzfeld [22] (p. 612 and following; see also [14]).

**) According to Unsöld [19] and Regemorther [13]. The measurements of Schütz [18] add on new result.

values. This supposition becomes still more probable when a comparison is made with analogous plots for other alkali elements, since these plots have almost the same shape, with no sudden bends.*) In consequence of unexpected unreliability of the $f_6, \ldots, f_{15}$ values of Cs, further calculations have been performed in two versions: A) using the unchanged values of Waibel, and B) multiplying them by 10. Results are given in Table I, together with experimental data.**) Fig. 2

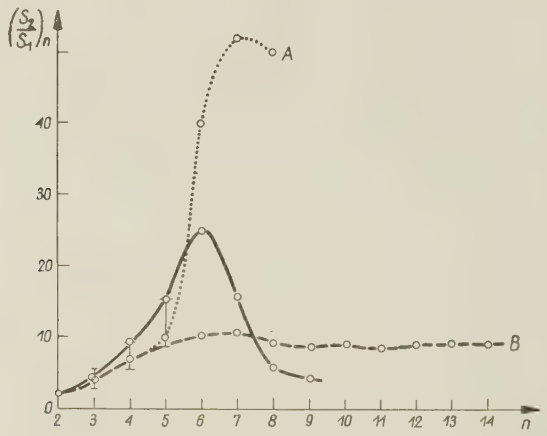

Fig. 2. Plot of $(S_2/S_1)_n$ against n

gives $(S_2/S_1)_n$ plotted against n. The dotted and dashed lines refer to the versions A) and B), respectively. The plot A) has a strange break near $n = 6$; the perturbation correction becomes in this case so large that the use of formula (1) seems no more legitimate for $n \geqslant 9$. On the contrary, the assumption B) leads to a smooth curve. For precautions sake one must still admit a possibility of $f_6, \ldots, f_{15}$ being contained between these two alternative sets of values, but if so, one may expect them rather to approach the corrected values of version B). In this case the plot of Fig. 2 would preserve the shape of the dashed curve, passing, however, somewhat above it for $n \geqslant 6$. The full line connects experimental values of Sambursky [16]. Vertical segments indicate the range of other experimental results (except those of Beutell [2] for $n = 6$ and 7, as the latter lie far beyond the scale of Fig. 2).

The results of Sambursky and Beutell are thus quite contradictory for $n \geqslant 6$. The present author's theoretical values follow neither the first, nor the second alternative. They seem, however, to be in good accord with a remark made by Kratz [10], at the end of his paper: although no quantitative intensity measurements have been made by the latter, he suggests, after the inspection of his plates that relative doublet intensities for the principal series of Cs show steady increase, perhaps

*) One may use for this purpose the results of Filippov and Prokofiew [5] for Na. Similar plots might be obtained for K and Rb, but less f-values are known for these elements.

**) The $(\nu_2/\nu_1)^4$-correction has been introduced into the measured intensities.

to an asymptotic value. Almost the same behaviour has been theoretically predicted on the basis of general consideration for one-electron spectra by Sambursky [17] (contradicting his own earlier experimental results for Cs [16]). After a provisional estimation of lim $(F_n - F_{n-1})$, F_n being given by (2), he suggests an asymptotic increase of $(S_2/S_1)_n$, preceeded perhaps by a local maximum and minimum in the neighbourhood of $n = 7$ (caused by the non-hydrogenlike character of the alkali terms). Some flat extrema on the dashed curve, and its subsequent asymptotic hebaviour seem to be present in Fig. 2. It must, however, be remembered that errors resulting from the inaccuracy of experimental f-values are nearly of the same magnitude for further members of the series. Obviously, the existence of such extrema could not be predicted by the qualitative observation of Kratz.

New, more accurate measurements of relative doublet intensities for further members of the series would be necessary for a conclusive accuracy test of the Fermi formula for them. At the same time a more precise knowledge of the corresponding f-values would provide a still better evaluation of Eq. (1). Calculations similar to those, given here for Cs would be possible also for Na, owing to the many f-values known for this element.

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TABLE I

Values of f_n, ϱ_n^2 and $\left(\frac{S_1}{S_2}\right)_n$

Author	n		2	3	4	5	6	7	8	9	10	11	12	13	14	15
Roschdestvensky Füchtbauer (exp.)	f_n		1	1.6×10^{-2}	2.7×10^{-3}	8.0×10^{-4}										
Minkowski Mühlenbruch (exp.)	f_n		1	1.45×10^{-2}												
Waibel (exp.)	f_n		—	—	—	—										
	f_n	A	1	$1.5\cdot10^{-2}$	$2.7\cdot10^{-3}$	$8.0\cdot10^{-4}$	$3.9-\begin{cases}10^{-5}\\10^{-5}\\10^{-4}\end{cases}$	$2.3\times\begin{cases}10^{-5}\\10^{-5}\\10^{-4}\end{cases}$	$1.8\times\begin{cases}10^{-5}\\10^{-5}\\10^{-4}\end{cases}$	$1.4\times\begin{cases}10^{-5}\\10^{-5}\\10^{-4}\end{cases}$	$1.0\times\begin{cases}10^{-5}\\10^{-5}\\10^{-4}\end{cases}$	$8.1\times\begin{cases}10^{-6}\\10^{-6}\\10^{-5}\end{cases}$	$6.2\times\begin{cases}10^{-6}\\10^{-6}\\10^{-5}\end{cases}$	$4.9\times\begin{cases}10^{-6}\\10^{-6}\\10^{-5}\end{cases}$	$3.9\times\begin{cases}10^{-6}\\10^{-6}\\10^{-5}\end{cases}$	$3.0\times\begin{cases}10^{-6}\\10^{-6}\\10^{-5}\end{cases}$
		B														
Combined experimental results	log $(10^6 f_n)$	A	6	4.18	3.43	2.90	1.59	1.36	1.26	1.14	1.00	0.91	0.79	0.69	0.59	0.48
		B					2.59	2.36	2.26	2.14	2.00	1.91	1.79	1.69	1.59	1.48
	ϱ_n^2	A	1	7.7×10^{-3}	1.2×10^{-3}	3.3×10^{-4}	$1.6\times\begin{cases}10^{-5}\\10^{-4}\end{cases}$	$9.0\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$6.9\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$5.4\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$3.9\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$3.1\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$2.3\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$1.8\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$1.5\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$	$1.1\times\begin{cases}10^{-6}\\10^{-5}\end{cases}$
		B														
Gentile Maiorana (theor.)	ϱ_n^2		1	8.0×10^{-3}												
Bates Damgaard (theor.)	ϱ_n^2		1	1.3×10^{-2}	(2.7×10^{-3})											
Calculated after formula (1)	$\left(\frac{S_2}{S_1}\right)_n$	A	2.0	4.0	6.8	10.0	40	52	50	—	—	—	—	—	—	—
		B	2.0	4.0	6.7	9.0	10.3	10.7	9.4	8.7	9.0	8.5	9.0	9.2	9.2	—
Sambursky (exp.)	$\left(\frac{S_2}{S_1}\right)_n$		—	4.5	9.6	15.5	25.0	15.8	5.7	4.5						
Other experim. results cited after Beutell	$\left(\frac{S_2}{S_1}\right)_n$		2	3.3—5.5	5.6—8.7	9.1—15.6										
Beutell	$\left(\frac{S_2}{S_1}\right)_n$		—	4.1	8.7	15.6	50—80	110—170								

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Electrons and Holes in Indium Antimonide

by
J. KOŁODZIEJCZAK

Presented by L. SOSNOWSKI on January 13, 1961

The carrier distribution in the various energy bands is determined by the value of the Fermi level; the latter, in turn, is determined by the concentration of impurities in the sample and by the state densities in the bands. If N_d denotes the concentration of donors and P_a — that of acceptors, the concentration of free electrons from the impurity amounts to $n_d = N_d - P_a$. According to results obtained by Baltensperger [1], at sufficiently high concentrations of the impurities, the discrete impurity level splits yielding a band that can coincide with the conductivity band. In the case of InSb, because of the small effective mass of the electrons, this occurs already at a donor concentration of the order of 10^{14} cm.$^{-3}$. This phenomenon accounts for the absence of an activation energy and, thus, for the fact that a constant concentration of free electrons (amounting to $n_d = N_d - P_a$) is kept up even at the lowest temperatures.

This gives rise to strong degeneracy of the electron gas in InSb. At thermodynamical equilibrium, the following condition is fulfilled:

$$n = p_1 + p_2 + n_d \tag{1}$$

with n denoting the total electron concentration in the conductivity band, and p_1, p_2 — the concentration of heavy and light holes in the corresponding valence bands, respectively. According to Kane's results [2], the conductivity band and that of the light holes are non-parabolic bands, whereas that of the heavy holes can be considered to be parabolic. Kane's results are correct at the temperature of absolute zero. As modified for higher temperatures, the energy bands in InSb are of the form

$$\begin{cases} \varepsilon_c = \dfrac{\hbar^2 k^2}{2m_0} + \dfrac{1}{2}\left\{\left(\varepsilon_g^2 + \dfrac{8}{3}P^2 k^2\right)^{1/2} - \varepsilon_g\right\}, \\ \varepsilon_{v_1} = -\dfrac{\hbar^2 k^2}{2m_{v_1}^*} - \varepsilon_T, \\ \varepsilon_{v_2} = -\dfrac{\hbar^2 k^2}{2m_0} - \dfrac{1}{2}\left\{\left(\varepsilon_g^2 + \dfrac{8}{3}P^2 k^2\right)^{1/2} - \varepsilon_g\right\} - \varepsilon_T. \end{cases} \tag{2}$$

This modification consists in taking into account the dilatation of the crystal lattice and the interaction between the electrons and the phonon field. According to earlier results [3]—[5], the concentrations of the carriers in the various energy bands are given by the expressions

$$(3)\qquad \begin{cases} n = 2\left(\dfrac{2\pi m_n k_0 T}{h^2}\right)^{3/2} \dfrac{2}{\sqrt{\pi}} \displaystyle\int_0^\infty f_0(x-\eta)(x+\beta x^2)^{1/2}(1+2\beta x)\,dx, \\ p_1 = 2\left(\dfrac{2\pi m_{v_1}^* k_0 T}{h^2}\right)^{3/2} \dfrac{2}{\sqrt{\pi}} \displaystyle\int_0^\infty f_0(x+\eta+\eta^*)\,x^{1/2}\,dx, \\ p_2 = 2\left(\dfrac{2\pi m_{v_2} k_0 T}{h^2}\right)^{3/2} \dfrac{2}{\sqrt{\pi}} \displaystyle\int_0^\infty f_0(x+\eta+\eta^*)(x+\beta x^2)^{1/2}(1+2\beta x)\,dx, \end{cases}$$

where m_n, $m_{v_1}^*$, m_{v_2} are the effective masses of the electrons and of the holes of either kind in the lowest energy states of the various bands. Cyclotron resonance measurements yielded for m_n a value of 0.013 m_0 at low temperatures [6] and one of 0.015 m_0 at high temperatures [7]. For m_{v_1}, a value of 0.18 m_0 was obtained [6]. From the shape of the energy bands, m_{v_2} is equal to m_n. The distribution functions of the electrons and holes are as follows:

$$(4)\qquad \underbrace{f_0(x-\eta) = \frac{1}{1+e^{x-\eta}}}_{\text{electrons}} \qquad \underbrace{f_0(x+\eta+\eta^*) = \frac{1}{1+e^{x+\eta+\eta^*}}}_{\text{holes}},$$

where

$$x = \frac{\varepsilon}{k_0 T}, \qquad \eta = \frac{\zeta}{k_0 T}, \qquad \eta^* = \frac{\varepsilon_T}{k_0 T}, \qquad \beta = \frac{k_0 T}{\varepsilon_g},$$

ζ denoting the Fermi level with regard to the bottom of the conductivity band, ε_T the energy gap dependent on the temperature as a result of dilatation of the crystal lattice and interaction of the electrons with the phonon field, and ε_g — the energy gap as dependent on the temperature through dilatation of the crystal lattice only [3]. The temperature variation of ε_T was determined by means of infrared absorption measurements [8]. The temperature variation of ε_g is weaker than that of ε_T and, according to Ehrenraich, is given by $\partial\varepsilon_g/\partial T = -9.6\times10^{-5}$ eV/°K. At absolute zero both quantities are equal, amounting to 0.23 eV. With the foregoing experimental data, and taking into account that the various concentrations are given by the relations (3), Eq. (1) can be solved with respect to ζ. The solution for various concentrations of the impurities is shown in Fig. 1. At impurity concentration 10^{17} cm.$^{-3}$ the electron gas is strongly degenerate, as the Fermi level lies within the conductivity band throughout the entire temperature interval. For these concentrations, the intrinsic region can not be attained any more. By taking into account in (3) the Fermi level thus computed, the various concentrations can be evaluated.

The results are given in Figs. 2 and 3. It is of interest to make a comparison with the experimental results: this has been done for the intrinsic case. The upper graph

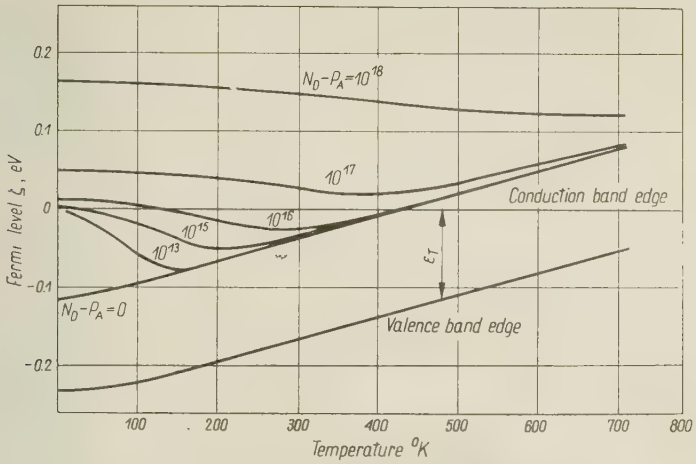

Fig. 1. Temperature dependence of Fermi level in *n*-type InSb with different concentrations of impurities

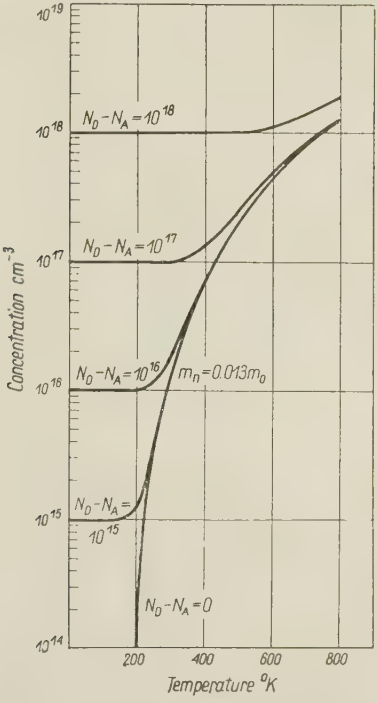

Fig. 2. Graph of electron concentration in *n*-type InSb with different concentrations of impurities computed for $m_n = 0.013\, m_0$

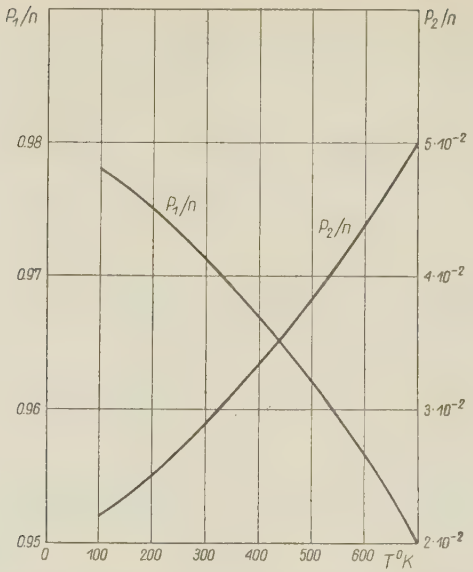

Fig. 3. Ratio of concentration of heavy holes to that of electrons, and of concentration of light holes to that of electrons, versus the temperature; intrinsic case

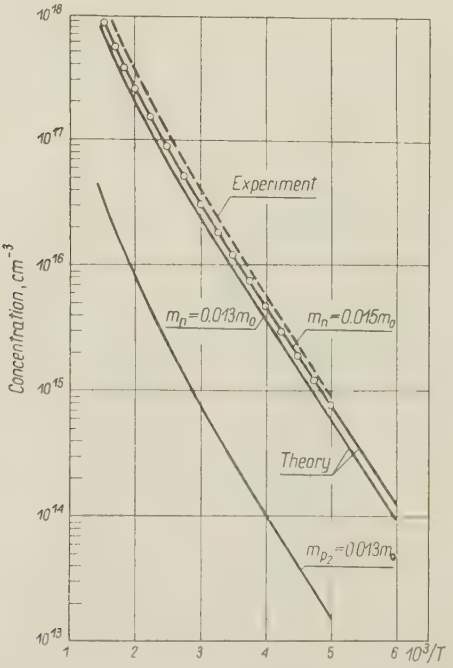

Fig. 4. Lower graph — Concentration of light holes versus the temperature. Upper graph — intrinsic concentration of electrons computed for $m_n = 0.013\ m_0$ and $m_n = 0.015\ m_0$

in Fig. 4 shows the intrinsic concentration of electrons as computed for $m_n = 0.013\ m_0$ and $m_n = 0.015\ m_0$. The dashed curve is that of the experimental results due to Hrostowski [9] and Putley [10]. The foregoing concentration was determined from the formula of Hall's constant taking into account only one kind of carriers, i.e. neglecting the effect of the holes of either kind on this constant. The strict analysis on the assumption that the mobility of the light holes is equal to that of the electrons, in the intrinsic case, leads to the following relations for Hall's constant:

$$R = -\frac{3\pi}{8}\frac{1}{en_i}\frac{\frac{p_1}{n}(b^2-1)}{\left[2b-\frac{p_1}{n}(b-1)\right]^2}, \tag{5}$$

where b is the ratio of the mobility of the electrons and that of the heavy holes. It is known from the literature, that this ratio varies within very wide limits. Its mean value, as obtained from a considerable number of measurements of different samples, amounts to 27 [11]. If the intrinsic concentration n_i is determined from

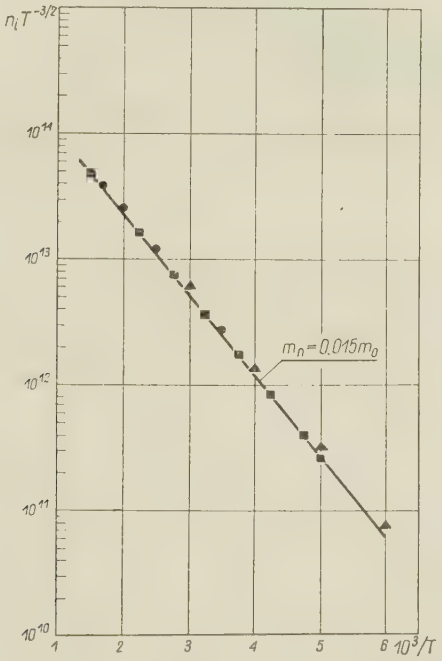

Fig. 5. Graph of $nT^{-3/2}$ *versus* $1/T$. Continuous curve — theoretical points; experimental values according to: ● Hrostowski, ▲ Putley, ■ Welker

Eq. (5), the results of Hrostowski and Putley yield points coinciding with the theoretical curve as computed for $m_n = 0.015\ m_0$. These are denoted by dots in Fig. 4., Fig. 5 shows the dependence of $n.T^{3/2}$ on $1/T$. It is noteworthy that, notwithstanding

the high degree of complication of the assumptions made in evaluating the concentration, the graph is obtained in the form of a straight line. An interpretation of the experimental results on a basis of the simplest theory with the intrinsic concentration in the form

$$n_i = 2\left(\frac{2\pi m_n k_0 T}{h^2}\right)^{3,2} e^{-\frac{\varepsilon_T}{2k_0 T}} \tag{6}$$

would lead to an energy gap of 0.27 eV as obtained from the slope of the straight line in Fig. 5, a result obviously in contradiction with the results of absorption measurements. This contradiction is eliminated when the structure of the energy bands is taken into account.

The author wishes to thank Professor L. Sosnowski for his interest in the present investigation and for his critical remarks and valuable discussions.

Summary

On the basis of Kane's results relating to the energy band structure in InSb, the author evaluated the concentrations of electrons, heavy holes and light holes throughout the temperature range of 200°K to 700°K and for different concentrations of the impurities. The values of the intrinsic concentration computed are in good agreement with the experimental results.

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BULLETIN DE L'ACADÉMIE
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On the Most Cartesian-like Co-ordinate System

by

L. INFELD

Presented on February 6, 1961

Introduction

In the General Relativity Theory one usually assumes four co-ordinate conditions. The common ones are of the form

$$((-g)^W g^{\alpha\beta})_{|\alpha} = 0 . \tag{1}$$

For $W = 1/2$ this is the de Donder condition. In the case of motion of singularities and the investigation of gravitational radiation we find it convenient to use the following co-ordinate condition (Greek letters run from 0 to 3. Latin from 1 to 3, stroke denotes differentiation)

$$\begin{aligned} ((-g)^{1/2} g^{0\beta})_{|\beta} &= 0 , \\ ((-g)^{1,2} g^{mn})_{|n} &= 0 . \end{aligned} \tag{2}$$

We will try to formulate the problem of finding a most Cartesianlike co-ordinate system in mathematical terms. We shall see whether in this way we obtain co-ordinate conditions resembling (1).

The variational principle

Let us assume all our singularities enclosed by a space surface S not to be transgressed by our bodies between the "times" $x^{0'}$ and $x^{0''}$. We assume further that at infinity our co-ordinate system is Cartesian. That is

$$g^{\alpha\beta} = \eta ; \qquad \eta^{00} = 1, \qquad \eta^{0n} = 0, \qquad \eta^{mn} = -\delta^{mn} . \tag{3}$$

As we know, four arbitrary non tensorial co-ordinate conditions may be introduced. We ask: for what conditions does our system become Cartesian-like as rapidly as is possible outside S? The deviation of the co-ordinate system from the Cartesian is characterized by

$$h^{\alpha\beta} = g^{\alpha\beta} - \eta^{\alpha\beta} \tag{4}$$

or

$$\gamma^{\alpha\beta} = \sqrt{-g}\, g^{\alpha\beta} - \eta^{\alpha\beta} . \tag{5}$$

The first question we ask ourselves is — what independent quasi-scalar expressions can characterize the deviation of our system from the Cartesian? By quasi-scalar we understand expressions that would be scalar in a Minkowski space. The most simple expressions not involving derivatives are

$$A = \int [(-g)^W - (-g)^{1/2}]\, d_4x, \tag{6a}$$

$$B = -\frac{1}{4} \int (-g)^W h^{\alpha\beta} h_{\alpha\beta}\, d_4x. \tag{6b}$$

(The — sign is to make (6b) positive definite since the leading terms in $h_{\alpha\beta}$ are negative and in $h^{\alpha\beta}$ positive). Both become zero in a Euclidean space and in a Cartesian co-ordinate system. Varying these expressions independently with respect to small changes of the co-ordinate system we would obtain more co-ordinate conditions than allowed. Therefore, let us multiply one of them by λ and add it to the other. Thus we shall discuss the variation of

$$\lambda A + B = \lambda \int [(-g)^W - (-g)^{1/2}]\, d_4x - \frac{1}{4} \int (-g)^W h_{\alpha\beta} h^{\alpha\beta}\, d_4x, \tag{7}$$

where the integration is taken from S to infinity and from $x^{0'}$ to $x^{0''}$. Varying the co-ordinate system we shall use the formulae

$$\begin{cases} -\delta g^{\alpha\beta} = g^{\alpha\mu}\xi^{\beta}_{|\mu} + g^{\beta\mu}\xi^{\alpha}_{,\mu} - g^{\alpha\beta}_{|\mu}\xi^{\mu} \\ \delta g_{\alpha\beta} = g_{\alpha\mu}\xi^{\mu}_{|\beta} + g_{\beta\mu}\xi^{\mu}_{|\alpha} + g_{\alpha\beta|\mu}\xi^{\mu}, \end{cases} \tag{8}$$

where

$$\xi^k = x^k - x^{|k}.$$

First we shall vary (6a):

$$\delta A = \delta(-g)^W d_4x = -\int W(-g)^W g_{\alpha\beta}\delta g^{\alpha\beta} d_4x = \tag{9}$$

$$= (1-2W)\int [(-g)^W]_{|\mu}\xi^{\mu}\, d_4x,$$

since ξ vanishes at the end of integration limits. Let us vary (6b) remembering that in this approximation when we neglect h^2, we have

$$\begin{cases} h^{00} = -h_{00}, \qquad h^{ks} = -h_{ks}, \\ h^{0m} = h_{0m}. \end{cases} \tag{10}$$

Since we are not interested in the products of h's it is sufficient to use the formula

$$\begin{cases} \delta g_{00} = 2\xi^0_{|0}, \\ \delta h_{0n} = \xi^1_{|n} - \xi^n_{|0}, \\ \delta h_{mn} = -\xi^m_{|n} - \xi^n_{|m}, \end{cases} \tag{11}$$

which follows from (8).

Therefore in our approximation we obtain

$$\delta B = -\frac{1}{2} \int (-g)^W h^{\alpha\beta}\delta h_{\alpha\beta}\, d_4x = \int (-g)^W (\xi^0 h^{\alpha 0}_{\ |\alpha} - \xi^s h^{s\alpha}_{\ |\alpha})\, d_4x. \tag{12}$$

Retaining linear terms we have by varying (7) and assuming that the variation vanishes

$$\lambda(1-2W)[(-g)^W]_{|\mu}\,\xi^\mu + (-g)^W(\xi^0 h^{\alpha 0}_{|\alpha} - \xi^s h^{s\alpha}_{|\alpha}) = O(h^2). \tag{13}$$

Therefore for

$$\lambda = (1-2W)^{-1}$$

we have

$$((-g)^W g^{\alpha\beta})_{|\beta} = O(h^2). \tag{14}$$

Therefore (14) is identical with (1) if we consider only linear terms. For $W = 1/2$ (or $\lambda \to \infty$) we obtain in particular de Donder's condition. If we introduce γ in place of the h's, the de Donder condition becomes

$$\gamma^{\alpha\beta}_{|\beta} = O(\gamma^2). \tag{15}$$

From now on we assume additionally — to the end of this paper:

$$\gamma^{\alpha\beta} \to 0 \quad \text{at least like} \quad \frac{1}{r} \quad \text{for } r \to \infty, \tag{16}$$

where

$$r^2 = x^k x^k$$

or

$$|\gamma^{\alpha\beta}| \leqslant \left| \frac{M_{\alpha\beta}(x_0)}{r} \right|, \text{ for } r \to \infty. \tag{17}$$

Therefore all space derivatives of $\gamma_{\alpha\beta}$ are of the order $(1/r^2)$ and the time derivatives are of the order $1/r$ and so we can write de Donder's condition in the form

$$\gamma^{\alpha\sigma}_{|\sigma} = O\left(\frac{M^2}{r^2}\right) \quad \text{everywhere outside } S. \tag{18}$$

It is equally simple to obtain the condition

$$\begin{cases} \gamma^{0\sigma}_{\sigma} = O\left(\dfrac{M^2}{r^2}\right), \\ \gamma^{mn}_{n} = O\left(\dfrac{M^2}{r^3}\right). \end{cases} \tag{19}$$

The only difference in the procedure is that we shall now vary the same integral as before, assuming $\xi^k = \xi^k(x^l)$, but $\xi^0 = \xi^0(x^\mu)$ as before, that is ξ^k depends only on the space co-ordinates but ξ^0 on all co-ordinates.

It would appear that $\gamma^{\sigma 0}_{\sigma}$ is of a different order than γ^{kl}_{l}. However, this is not so, because it follows from $\gamma^{kl}_{l} = O(M^2/r^3)$ that γ^{00} must be of the form $4M/r$, where M is a constant [1]. Therefore γ^{00}_{0} is of order M/r^3. Since the neglected terms are products of the γ's and their derivatives, we have, finally,

$$\begin{cases} \gamma^{\sigma 0}_{1\sigma} = O\left(\dfrac{M^2}{r^3}\right), \\ \gamma^{mn}_{1n} = O\left(\dfrac{M^2}{r^3}\right). \end{cases} \tag{20}$$

Assuming these conditions, we annihilate gravitational radiation. This is an essential advantage over de Donder's condition.

This paper arose from my seminar discussions with Dr. Plebański. I would like to thank Mr. Mielnik and my son Eric for many pleasant discussions and for their help in formulating this paper.

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A Possible Mechanism of the $D_{3/2}$ $T = 1/2$ Resonance in Pion-Nucleon Scattering

by

W. KRÓLIKOWSKI

Presented by W. RUBINOWICZ on February 7, 1961

In [1] a possible mechanism of the inner D excitation of the nucleon was proposed in view of the higher resonances in pion-nucleon scattering. Within the last year the assigment $D_{3/2\ 1/2}$ for the second $\pi^- p$ resonance was experimentally confirmed, whereas the third $\pi^- p$ resonance turned out to be probably $F_{5/2\ 1/2}$ rather than $D_{5/2\ 1/2}$ [2].

The aim of the present note is to point out that the existence of the $D_{3/2\ 1/2}$ resonance and the simultaneous absence of any other D resonance would not be inconsistent with the mechanism proposed in [1].

To this end let us use formulae (10) and (11) in [1]. Assuming that the contribution from the state $J = 3/2$, $T = 1/2$ predominates over other D states in integrals I_{JT} and J_{JT} we get approximately the following formulae for D effective ranges:

$$\text{(1)} \qquad \begin{cases} r_{31}^D \approx \dfrac{14}{16}\dfrac{J_{31}}{I_{31}} > 0, \\ r_{33}^D \approx -\dfrac{J_{31}}{I_{31}} < 0, \\ r_{51}^D \approx -\dfrac{J_{31}}{I_{31}} < 0, \\ r_{53}^D \approx -\dfrac{J_{31}}{I_{31}} < 0. \end{cases}$$

The signs of r's are consistent with the above mentioned possibility.

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On the Final-State Interaction in Single-Pion Production Processes

by

A. KRZYWICKI

Presented by L. INFELD on February 14, 1961

It is known at present, that for energy of the incident pion being close to 1 Bev, the experimental data concerning the reaction $\pi^- + p \to \pi^- + \pi^+ + n$ are consistent with the isobar theory, while those concerning the reaction

$$\pi^- + p \to \pi^- + \pi^0 + p$$

demonstrate the importance of the process symbolised by the diagram in Fig. 1 [1]—[5]. It was pointed out, especially by Selleri, that this situation can be understood if we assume the existence of the final-state pion-nucleon resonant interaction. The simplest field-theoretical model, taking into account the rescattering of the produced pion, is that which starts from the diagram shown in Fig. 2, where the vertex E can be symbolically expressed in the following manner:

(1) 

In the case when the rescattering cross-section is small, the diagram in Fig. 2 is practically equivalent to the diagram in Fig. 1. When it is large, however, the processes symbolised by diagrams in Figs. 1 and 2, respectively, may have quite different features. In connection with the discussed model two problems arise. The

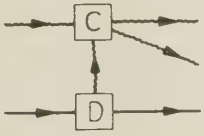

Fig. 1

first, of rather formal character, consists in finding a simple method for evaluating the matrix element corresponding to the rather complicated graph in Fig. 2. The second consists in comparing the predictions of the model with experiment. In

our communication we shall limit ourselves to the first problem. Since the calculational difficulties are connected with the interaction part of E (see (1)), we shall

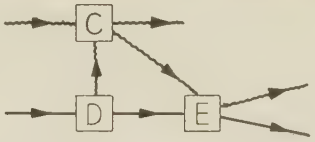

Fig. 2

calculate here only the matrix element and transition probability corresponding to the diagram in Fig. 3.

Let us observe (see Fig. 3) that the regions of integration with respect to k (internal line $C - T$) and t (internal line $D - T$) contain vicinities of poles corresponding to real meson and nucleon, respectively.

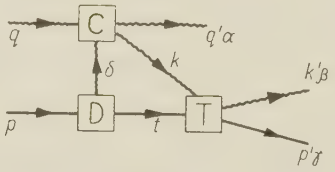

Fig. 3

In calculations we shall use the following simplifying assumptions:

a) Integrating with respect to k_0 and t_0 we shall assume that the major contribution comes from the vicinity of poles at $k_0 = (\vec{k}^2+\mu^2)^{1/2}$ and $t_0 = (\vec{t}^2+m^2)^{1/2}$, i.e. we make the following replacements under the appropriate integrals:

$$(2)\qquad \begin{cases} \dfrac{1}{k_\nu^2+\mu^2-i\eta} \to \dfrac{i\pi}{2\sqrt{\vec{k}^2+\mu^2}}\,\delta(k_0-\sqrt{\vec{k}^2+\mu^2}), \\ \dfrac{-i\,t_\nu\,\gamma^\nu+m}{t_\mu^2+m^2-i\eta} \to \dfrac{i\pi m}{\sqrt{\vec{t}^2+m^2}}\,\Lambda_+(\vec{t})\,\delta(t_0-\sqrt{\vec{t}^2+m^2}), \end{cases}$$

where $\Lambda_+(\vec{t})$ is the usual projection operator for states of positive energy. Thus, the vertex T can be expressed in terms of pion-nucleon phase shifts.

b) We replace the vertex C describing the virtual pion-pion scattering by the analogous quantity corresponding to the real pion-pion scattering, i.e. we put

$$(3)\qquad C[(q_\nu+\delta_\nu)^2, (q_\nu-q'_\nu)^2, \delta_\nu^2] \to C[(q_\nu+\delta_\nu)^2, (q_\nu-q'_\nu)^2, -\mu^2].$$

c) We assume that pion-pion and pion-nucleon scatterings at vertices C and T respectively are resonance-like scatterings.

d) For simplicity we assume that at the vertex T only 3/2, 3/2 isobar is produced. Generalisation is straightforward.

e) We calculate the vertex D using perturbation theory.

The matrix element corresponding to the diagram in Fig. 3 is (we neglect the constant phase factor):

$$(4)\quad M = \frac{\varrho}{V^{5/2}}\left(\frac{m^2}{8\,p_0\,q_0\,p_0'\,q_0'\,k_0'}\right)^{1/2}\int \cdot\, d_4\,\delta\, d_4\,k\, d_4\,t\,\bar{w}_s(\vec{p}')\cdot T\cdot$$

$$\times\frac{-i\,t_\nu\gamma^\nu + m}{t_\mu^2 + m^2 - i\eta}\cdot D\cdot w_r(\vec{p})\cdot\frac{1}{\delta_\sigma^2+\mu^2 - i\,\eta}\cdot\frac{1}{k_\nu^2+\mu^2 - i\eta}\cdot C\times$$

$$\times\,\delta_4(q+\delta-q'-k)\,\delta_4(p-\delta-t)\,\delta_4(k+t-k'-p').$$

ϱ depends only on the isotopic properties of the pion-pion interaction and charges of particles.

$$\varrho = (11,-10/11\,J-1)(11\,\alpha,\beta+\gamma-\tfrac{1}{2}/11\,J,-1)(1\tfrac{1}{2},\beta+\gamma-\tfrac{1}{2},\tfrac{1}{2}/1\tfrac{1}{2}J',\beta+\gamma)\times$$

$$\times(1\tfrac{1}{2}\,\beta\gamma/1\tfrac{1}{2}J',\beta+\gamma)+\sqrt{2}\,(11,-11/11\,JO)(11\alpha,\beta+\gamma+\tfrac{1}{2}/11\,J0)\times$$

$$\times(1\tfrac{1}{2},\beta+\gamma+\tfrac{1}{2},-\tfrac{1}{2}/1\tfrac{1}{2}J'\,\beta+\gamma)(1\tfrac{1}{2}\,\beta\gamma/1\tfrac{1}{2}J',\beta-\gamma),(\alpha+\beta+\gamma=-\tfrac{1}{2}).$$

J and J' are isotopic spins of pion-pion and pion-nucleon isobars respectively, Greek indices correspond to third components of isospin of final particles. V is the normalisation volume. The meaning of other symbols can be read in Fig. 3.

We can write

$$(5)\qquad T = -A + i\,Q_\nu\,\gamma^\nu\,B,$$

where

$$Q_\nu = \tfrac{1}{2}(k_\nu + k_\nu').$$

From a) and b) it follows that

$$A = A\,[(p_\nu'+k_\nu')^2,(k_\nu'-k_\nu)^2]$$
$$B = B\,[(p_\nu'+k_\nu')^2,(k_\nu'-k_\nu)^2]$$
$$C = C\,[(q_\nu+\delta_\nu)^2,(q_\nu'-q_\nu)^2].$$

Using our assumptions a), b), e) we perform the integrations with respect to k, t and δ_0 by means of δ-functions. At the moment we do not care about the restrictions concerning the remaining variables which we get as a result of our integrations. Thus, the integration volume Ω in the formula below is not yet specified. We shall return to this problem later.

Thus,

$$(6)\quad M = \frac{\pi^2\,gm^2\,\varrho}{V^{5/2}(8\,p_0\,q_0\,p_0'\,q_0'\,k_0)^{1/2}}\,\delta_3(\vec{p}+\vec{q}-\vec{q}'-\vec{k}'-\vec{p}')\times$$

$$\times\int_\Omega d_3\vec{\delta}\,\{\bar{w}_s(\vec{p}')\,[-A+iQ_\nu\gamma^\nu B]\,\Lambda_+(\vec{p}-\vec{\delta})\gamma^5\,w_r(\vec{p})\}\times$$

$$\times\frac{C}{2\sqrt{(\vec{p}-\vec{\delta})^2+m^2}\cdot\sqrt{(\vec{q}+\vec{\delta}-\vec{q}')^2+\mu^2}\cdot(\delta_\mu^2+\mu^2)}$$

$$\times\,\delta_0(q_0+p_0-q_0'-\sqrt{(\vec{p}-\vec{\delta})^2+m^2}-\sqrt{(\vec{q}+\vec{\delta}-\vec{q}')^2+\mu^2})\times$$

$$\times\,\delta_0(\sqrt{(\vec{q}+\vec{\delta}-\vec{q}')^2+\mu^2}+\sqrt{(\vec{p}-\vec{\delta})^2+m^2}-k_0'-p_0').$$

We pass to the cms ($\vec{p}+\vec{q}=0$) and introduce a new integration variable $\vec{s}=\vec{q}+\vec{\delta}'$.

In order to perform the last intergrations we choose the co-ordinate axes for $\vec{s}$ in the manner shown in Fig. 4. Using the δ-function under the integral in (6) we integrate with respect to cos θ

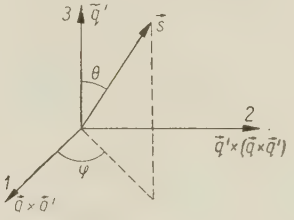

Fig. 4

$$(7)\qquad M=\frac{m^2\pi^2 g\varrho}{V^{5/2}q'(8p_0q_0p_0'q_0'k_0')^{1/2}}\delta_4(p+q-p'-q'-k')\times$$

$$\times\int\limits_{\Omega'}ds\,d\varphi\,\frac{{}^{I}s\,C}{2\sqrt{s^2+m^2}\,(\delta_\nu^2+\mu^2)}\{\bar{w}_s(\vec{p}')[-A+iQ_\mu\gamma^\mu B]\times$$

$$\times\Lambda_+(-\vec{s})\gamma^5 w_r(\vec{p})\}.$$

In $\Lambda_+(-\vec{s})$ the angle between $\vec{s}$ and $\vec{q}'$ is fixed by the last integration and δ_ν^2 is a function of s and φ. One can verify that in (7)

$$(8)\qquad C=C[(s^2-(q_0+p_0-\sqrt{s^2+m^2})^2),(q_\nu'-q_\nu)^2],$$

i.e. C is independent of φ. Clearly s is connected with the mass V_0 of the pion-pion isobar by the equation

$$(9)\qquad \sqrt{s^2+m^2}=\frac{(p_0+q_0)^2+m^2-V_0^2}{2(p_0+q_0)}.$$

Let us denote by $\tilde{V}_0$ the mass of the pion-pion isobar corresponding to the maximum in pion-pion cross-section and by $\tilde{s}$ the quantity given by (9) when $V_0=\tilde{V}_0$. C has a rapid maximum at $s=\tilde{s}$ and the propagator $(\delta_\nu^2+\mu^2)^{-1}$ is large only when the deflection of the nucleon at the vertex D is small.

Thus

$$(10)\qquad M\approx\frac{\pi^2 m^2 g\varrho}{V^{5/2}\cdot 4q'(p_0+q_0)(8p_0q_0p_0'q_0'k_0')^{1/2}}\delta_4(p+q-q'-p'-k')\times$$

$$\times\{\bar{w}_s(\vec{p}')[-A+iQ_\nu\gamma_\nu^* B]\Lambda_+(-\vec{s})\gamma^5 w_r(\vec{p})\}_{\substack{s=\tilde{s}\\ \vec{s}\,|\,\vec{q}}}\cdot I_{(1)}\cdot I_{(2)},$$

where

$$I_{(1)} = \frac{1}{m^2} \int_{\Omega_1} C\,[V_0^2,\ (q_\nu - q'_\nu)^2]\,dV_0^2$$

$$(11)\quad I_{(2)} = \int_{\substack{\Omega_2 \\ s=\tilde{s}}} \frac{m^2\,d\varphi}{(\delta_\nu + \mu^2)} \approx$$

$$\approx \int_{\Omega_2} \frac{d\varphi}{\left[\left(\frac{\mu}{m}\right)^2 + \left(\frac{p-\tilde{s}}{p_0}\right)^2 + \frac{2p\tilde{s}}{m^2}\,(1 - \cos\theta_0 \cos\theta_{q'} - \sin\theta_0 \sin\theta_{q'} \sin\varphi)\right]}$$

$\cos\theta_{q'} = \dfrac{\vec{q}\cdot\dot{q}}{qq'}$ and θ_0 is defined by the equation

$$q_0 + p_0 - q'_0 - \sqrt{\tilde{s}^2 + m^2} - \sqrt{\tilde{s}^2 + q_0'^2 - 2\tilde{s}q' \cos\theta_0} = 0\,.$$

So far we did not care about the restrictions imposed both on the integration volume and phase space volume corresponding to final states, by performing the integrations using δ-functions occurring in the integrand of (4). The finding of the exact form of these restrictions needs very cumbersome calculations. We do not consider to be of much sense to do those calculations exactly, since the matrix element is obtained by a very approximate method. Fortunately, the form of the matrix element is such that we can attack the problem in a different way. Let us denote by χ the angle of deflection of the nucleon at the vertex D. Let us assume also that $|C|$ is appreciable when

$$V_0^{(1)} \leqslant V_0 \leqslant V_0^{(2)}.$$

One can verify that

$$\cos\chi = \cos\theta_0 \cos\theta_{q'} + \sin\theta_0 \sin\theta_{q'} \sin\varphi\,. \qquad \text{Since } \frac{2p\tilde{s}}{m^2} \geqslant \left(\frac{\mu}{m}\right)^2 + \left(\frac{p-\tilde{s}}{p_0}\right)^2$$

the contribution of the one-meson propagator corresponding to the internal line $C-D$ is large when $1 - \varepsilon \leqslant \cos\chi \geqslant 1$, where ε is of the order of magnitude of

$$\left[\left(\frac{\mu}{m}\right)^2 + \left(\frac{p-\tilde{s}}{p_0}\right)^2\right] \cdot 2 \cdot \frac{p\tilde{s}}{m^2}.$$

Making simple kinematical considerations we can find within what limits must lie $\vec{q}$ when $V_0^{(1)} \leqslant V_0 \leqslant V_0^{(2)}$ and $1 - \varepsilon \leqslant \cos\chi \leqslant 1$.

We introduce the following quantities σ, α, β:

$$(12)\quad \begin{cases} \sigma = [(p_0+q_0)^4 + (V_0^2 - m^2)^2 - 2(p_0+q_0)^2(m^2+V_0^2)]^{1/2}/2(p_0+q_0), \\ \alpha = \arccos\left\{\dfrac{V_0}{\sigma(p_0+q_0)(V_0^2-4\mu^2)^{1/2}} - \dfrac{[(p_0+q_0)^2+\mu^2-W^2-(\sigma^2+V_0^2)^{1/2}(p_0+q_0)]}{\sigma(V_0^2-4\mu^2)^{1/2}}\right\} \\ \beta = \operatorname{arc\,tg}\left\{\dfrac{V_0(V_0^2-4\mu^2)^{1/2}\sin(\alpha)}{(\sigma^2+V_0^2)^{1/2}\cdot(V_0^2-4\mu^2)^{1/2}\cos\alpha + \sigma V_0}\right\}. \end{cases}$$

(W denotes here the mass of the pion-nucleon isobar).

Let $\beta_{(W)}^{(\max)}$ and $\beta_{(W)}^{(\min)}$ be the maximum and minimum value of P for V_0 lying in the interval $(V_0^{(1)}, V_0^{(2)})$, and $\chi^{(max)} = \arccos(1-\varepsilon)$.

Then

$$\theta_{q'}^{(\min)} \leqslant \theta_{q'} \leqslant \theta_{q'}^{(\max)}, \tag{13}$$

where

$$\theta_{q'}^{(\max)} = \beta^{(\max)} + \chi^{(\max)}$$

$$\theta_{q'}^{(\min)} = \begin{cases} \beta^{(\min)} - \chi^{(\max)} & \beta^{(\min)} > \chi^{(\max)} \\ 0 & \beta^{(\min)} \leqslant \chi^{(\max)}. \end{cases}$$

We have also

$$q_0' = \sqrt{\vec{q}'^2 + \mu^2} = \frac{(p_0 + q_0)^2 + \mu^2 - W^2}{2(p_0 + q_0)}. \tag{14}$$

As it could be expected for fixed (p_0+q_0), the allowed region for q' is dependent on W only. This dependence is unfortunately complicated, but in practical calculations (when ε, $V_0^{(1)}$ and $V_0^{(2)}$ are fixed) it can be approximated by some simple one. The allowed region for $\vec{p}'$ and $\vec{k}'$ can be found by considering the "decay" of the excited nucleon with momentum $-\vec{q}'$ and mass W.

As an example of calculation of transition probability while taking into account final state interaction we shall calculate the transition probability P corresponding to the diagram in Fig. 3. Summing and averaging over final and initial polarization states respectively we find:

$$P \approx \frac{1}{2}(2\pi)^4 \frac{\pi 4\, \pi^4 m^4 g^2 \varrho^2}{V^4 q'^2 \cdot 16 (p_0+q_0)^2 \cdot (8 p_0 q_0 p_0' q_0' k_0')} \times \\ \times \delta_4(p+q-p'-q'-k') \cdot |I_{(1)}|^2 \cdot I_{(2)}{}^2 \cdot \mathcal{L}. \tag{15}$$

where

$$\mathcal{L} = T_r\{\gamma^5 \Lambda_+(-\hat{s})(A^* - iQ_\nu \gamma^\nu B^*) \Lambda_+(\hat{p}')(-A + iQ_\mu \gamma^\mu B) \times \\ \times \Lambda_+(-\vec{s}) \gamma^5 \Lambda_+(\vec{p})\}_{\substack{s=\tilde{s} \\ \vec{s} \parallel \vec{q}}}. \tag{16}$$

After strightforward algebra we get

$$\mathcal{L} = \frac{4}{(2m)^4}\{X_1 A^* A + X_2 B^* B - X_3 \operatorname{Re} AB^*\}, \tag{17}$$

where

$$\begin{cases} X_1 = m^2 \delta_\nu^2 - \frac{1}{2}\delta_\nu^2 (p_\mu' \delta^\mu) - \delta_\nu^2 (p_\mu p'^\mu) \\ X_2 = 2\delta_\nu^2 (Q_\mu p^\mu)(Q_\gamma p'^\gamma) - \frac{1}{2}\delta_\nu^2 Q_\mu^2 (p_\gamma' \delta^\nu) + \\ \qquad + \delta_\nu^2 (Q_\mu \delta^\mu)(Q_\gamma p'^\gamma) - \delta_\nu^2 Q_\mu^2 (p_\gamma p'^\gamma) - m^2 \delta_\nu^2 Q_\mu^2 \\ X_3 = 2m \delta_\nu^2 (Q_\mu p') + 2m \delta_\nu^2 (Q_\mu p^\mu) + m \delta_\nu^2 (Q_\mu \delta^\mu). \end{cases} \tag{18}$$

We expand $Xi|\delta_\nu^2$ in powers of δ and retain only the zero order term, which we express in terms of $\varkappa^2 = \frac{1}{4}(k_\nu' - k_\nu)^2$ and $\nu = -Q_\nu \cdot (t^\nu + p'^\nu)/2m$.

One finds that terms containing $\varkappa^2$ are negligible, so that finally we get

$$X_1 \approx 2m^2 \delta_\nu^2 \qquad X_2 \approx 2m^2 \nu^2 \delta_\nu^2 \qquad X_3 \approx -4m^2 \nu \delta_\nu^2 \tag{19}$$

$$(\nu = \nu_L - \varkappa^2/m \approx \nu_L, \qquad \nu_L = EW/m - m$$

and E denotes the total energy of the emitted nucleon in the isobar rest frame and is clearly a function of W only). One can express A and B in terms of pion-nucleon scattering phase shifts According to our assumption d) we consider only the δ_{33} phase shift to be important. Finally we get

$$(20) \qquad P \approx \frac{1}{V^4} \frac{\pi m^2 g^2 \varrho^2 \sigma_{3/2}(W)}{2^8 q'^2 (p_0 + q_0)^2 p_0 q_0 p'_0 q'_0 k'_0} \delta_4(p + q - q' - p' - k') |I_{(1)}|^2 \cdot I^2_{(2)} \times$$

$$\times \left\{ \delta_\nu^2 \left[3 \frac{W + m + \nu_L}{E + m} \left(1 - \frac{\varkappa^2}{2(E^2 - m^2)} \right) + \frac{W - m - \nu_L}{E - m} \right]^2 \right\}_{\substack{\tilde{s} = \tilde{s} \\ \tilde{s} \parallel \tilde{q}}}.$$

We have also:

$$(\delta_\nu^2)_{\substack{\tilde{s} = \tilde{s} \\ \tilde{s} \parallel \tilde{q}}} \approx m^2 \left(\frac{p - \tilde{s}}{p_0} \right)^2$$

$$\left(1 - \frac{\varkappa^2}{2(E^2 - m^2)} \right)_{\substack{\tilde{s} = \tilde{s} \\ \tilde{s} \parallel \tilde{q}}} = 1 + \frac{1}{E^2 - m^2} (m^2 - p'_0 \sqrt{\tilde{s}^2 + m^2} \cdot \tilde{s} p' \cos \theta_{p'}).$$

The region of integration Ω_2 in $I_{(2)}$ is such that $1 - \varepsilon \leqslant \cos \chi \leqslant 1$, so that when $\theta_{q'}$ is sufficiently small $\Omega_2 = (0, 2\pi)$.

From (20) one can easily get the distribution $\dfrac{\partial^4 \sigma}{\partial W \, \partial p' \, \partial \cos \theta_{q'} \cos \theta_{p'}}$ using (14). This distribution is similar to that of the isobar theory, but since we started from a specific mechanism of isobar formation P has certain particular features. One can see that both P and the allowed volume in phase space depend strongly on the width of the pion-pion resonance. Since we took into account the spin of the excited nucleon, P contains a factor which gives a correlation between final and initial nucleon momenta. The important advantage of our scheme of calculation is that one can easily incorporate here other pion-nucleon resonanses. The predictions of the discussed model, obtained by using the proposed method of calculation will constitute the content of a separate paper.

I should like to express my gratitude to Professor Z. Koba for stimulating discussions and for reading the manuscript.

After completing this work I got the paper by H. J. Schnitzer, entitled *Pion production and the second pion nucleon resonance*. In this paper the problem of the rescattering of the final pion is discussed, although for lower energies and by a method using the formalism of static theory. We hope, that our scheme of calculation, which fails for lower energies, but is reasonable for energies close to 1 Bev and higher, can be useful in further analysis of single pion production processes.

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THEORETICAL PHYSICS

Information as a Fundamental Notion of Statistical Physics

by

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Between statistical mechanics based exclusively on principles of dynamics and of the theory of probability on one hand, and macroscopic thermodynamics on the other, there is a gap which cannot be filled by any further development of mathematical methods. At any rate, this is true for systems with number N of particles of the order, say, of 10^{23}, and with energy of interaction between particles not vanishingly small with respect to the total energy of the system. The reason for this is exactly the same as that which makes the application of principles of mechanics alone to such systems impossible: namely absolute ignorance of the initial conditions of motion and impossibility of solving such a complicated equation of motion (in this case a partial differential equation with 10^{23} variables; reduction to a smaller number of variables is excluded by non-vanishing interactions).

This situation is well known of long (cf., e.g., [1], [2]), and many authors have proposed to add to axioms of dynamics and the probability theory some additional postulates, as the ergodic hypothesis, Krylov's good mixing principle [2], Tolman's postulate of equal a priori probability [3], the principle of detailed balance, etc. Recently there is even a tendency to call this branch of physics not "statistical mechanics" but "statistical thermodynamics" to stress the difference of approach between the former (which may be applied, e.g., for small N or, in the case of ideal gas, even for great N) and the theory with additional postulates which is of a more phenomenological character. On the other hand, the difference between ordinary macroscopic thermodynamics and statistical thermodynamics consists in the principal possibility of calculating by the latter the fluctuations of any order of physical quantities, in contrast to mean (expectation) values which only the former may give.

The present authors would like to draw attention to the possibility of a yet more abstract point of view than that of statistical thermodynamics in the above sense. It consists in abstracting from probability distributions and in considering only information connected with these distributions as well as expectation values

of physical quantities. Thus, in each state of the system to every physical quantity there correspond two values: a mean value and an information value (the latter may be considered as the logarithm of the "uncertainty" of this quantity, i.e. some global measure of fluctuation). In the classical case such a theory would be almost identical with macroscopic thermodynamics, because all physical quantities are functions of co-ordinates and momenta and in principle there is only one basic probability distribution, therefore only one information corresponding to the entropy of the system*).

In the quantum case, however, the situation is not so simple, there are essentially different probability distributions (on different Boolean rings, see below) for non-commuting physical quantities and, therefore, essentially different informations, etc. In most practical cases the differences between classical and quantum cases will be macroscopically imperceptible, but certainly not in all cases.

In the present note we do not yet try to construct such an "informational thermodynamics", we take only a preparatory step in this direction consisting in mathematical investigation of the relation between notions of probability and information. So far, all definitions of information were based on the notion of probability (cf. [5], [6]). We shall try to reverse this order, i.e. first to define information abstractly and only then, by its means — probability. This situation is very similar to that with the notion of expectation value. Expectation value of some random variable may also be defined abstractly without using the notion of probability (as some linear functional) and only by means of it probability distribution may be determined (problem known as the momentum problem). Similarly as in the latter case, for exact determination of probability distribution an infinite (in general) number of expectation values must be known, so (in general) only an infinite number of information values may give a probability distribution. Since in "informational thermodynamics" the notion of probability should not occur, it is convenient and methodologically necessary to find such a definition of information, in which the notion of probability does not intervene.

We start from the notion of the Boolean ring (or algebra) of events (consisting in obtaining some values in the measurement of a physical quantity, cf. e.g. [7], [8]). Boolean rings will be denoted by $A, B, C, \ldots$, their elements by $a, b, c, \ldots$, the zero element by 0, the unit elements by $1_A, 1_B, 1_C, \ldots$, the operation of Boolean union (joint) by $\cup$, the intersection (meet) by $\cap$, the difference by. Furthermore, let $[a_1, \ldots, a_n, A_1, \ldots, A_k]$ be the least subring of A, containing all elements $a_1, \ldots, a_n$ and all subrings $A_1, \ldots, A_k$ of the ring A, and let $a \cap A$ be the subring of A, consisting of all elements of A which are contained in its element a.

*) Contrary to recent usage, we do not consider words "information" and "entropy" as synonyms, but the latter as a special case of the former, i.e. entropy = information of energy. This corresponds to the intention of Clausius who invented the term "entropy" and said (cf. [4], p. 390): "Das Wort Entropie habe ich absichtlich dem Worte Energie möglichst ähnlich gebildet, denn die beiden Grössen, welche durch diese Worte benannt werden sollen, sind ihren physikalischen Bedeutungen nach einander so nahe verwandt, dass eine gewisse Gleichartigkeit in der Benennung mir zweckmässig zu sein scheint".

Let $\mathcal{H}$ be a class of finite *) Boolean rings satisfying the following conditions:

(i) If $A \in \mathcal{H}$ and B is a subring of A, then $B \in \mathcal{H}$.

(ii) For any $A \in \mathcal{H}$ there exists a ring $B \in \mathcal{H}$ such that A is a proper subring of B.

DEFINITION. *A real-valued regular function H defined on $\mathcal{H}$ is called information, if it has the following properties*:

I. Connection between information of rings and of their subrings. Let $A \in \mathcal{H}$ and let a, b be a pair of disjoint elements of A, $a \neq 0$, $b \neq 0$. Setting $A_1 = a \cap A$, $A_2 = b \cap A$, $A_3 = (a \cup b) \cap A$, $\widetilde{A}_1 = [a, (1_A \setminus a) \cap A]$, $\widetilde{A}_2 = [b, (1_A \setminus b) \cap A]$, $\widetilde{A}_3 = [a \cup b_1, (1_A \setminus (a \cup b)) \cap A]$, we have the equality $(H(A) - H(A_3))\, H(A_1)\, H(A_2) = (H(A) - H(A_1))\, H(A_2)\, H(A_3) + (H(A) - H(A_2))\, H(A_1)\, H(A_3)$.

II. Local character of information. Let $A, B \in \mathcal{H}$ and A_1, B_2 be a pair of subrings of A and B, respectively, such that there exists an isomorphism φ of A_1 onto B_1 satisfying the equality $H(C) = H(\varphi(C))$ for any subring C of A_1 (we say then that A and B are H-equivalent and write $A \widetilde{H} B$) and, further, $[1_{A_1} \cap A, 1_{A_1} \setminus 1_{A_1}] \widetilde{H} [1_{B_1} \cap B, 1_B \setminus 1_{B_1}]$. Then, setting $A_0 = [1_{A_1}, (1_A \setminus 1_{A_1}) \cap A]$, $B_0 = [1_{B_1}, (1_B \setminus 1_{B_1}) \cap B]$, we have the equality

$$H(A) - H(A_0) = H(B) - H(B_0).$$

III. Monotonity. If B is a proper subring of A, then $H(B) < H(A)$.

IV. Indistinguishability. The ring from $\mathcal{H}$ is said to be H-homogeneous, if for every automorphism ψ of A and for every subring B of A we have the equality $H(B) = H(\psi(B))$. We assume that isomorphic H-homogeneous rings are H-equivalent.

V. Normalization. Denoting the number of atoms (elementary events) of A by $N(A)$, we assume that, if $N(A) = 2$ and A is H-homogeneous, then $H(A) = 1$.

There holds the following

THEOREM. *If $H(A)$ is an information on $\mathcal{H}$, then for every $A \in \mathcal{H}$ there exists one and only one strictly positive probability measure p_A defined on A and such that for every subring B of A*

$$p_B(b) = \frac{p_A(b)}{p_A(1_B)} \qquad (b \in B)$$

and

$$H(A) = -\sum_{j=1}^{n} p_A(a_j) \log_2 p_A(a_j),$$

where $a_1, \ldots, a_n$ denote all atoms of A.

*) For the sake of simplicity we consider here only finite Boolean rings. The general case is discussed in [9].

A proof of the theorem as well as a more extensive mathematical discussion of our problem are given in [9].

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On the Antilinearization of the Klein-Gordon Equation for 4-Spinor

by

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1. Let us assume

$$\hat{D}^2(\partial_\mu, m) = \Box - m^2, \tag{1}$$

where $\hat{D}$ — scalar form. From (1) follows that

$$\hat{D}_1(\partial_\mu, m) = \gamma_\mu \partial_\mu \pm im\gamma_5 \tag{2a}$$

or

$$\hat{D}_2(\partial_\mu, m) = i\gamma_5(\gamma_\mu \partial_\mu \pm m), \tag{2b}$$

where

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \quad \{\gamma_\mu, \gamma_5\} = 0, \tag{3}$$

and moreover we can choose $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4$.

It is well-known that two forms ((2a) and (2b)) of operator are equivalent. Indeed, after the following interchange

$$\gamma_\mu \leftrightarrow i\gamma_5\gamma_\mu$$

allowed by (3), we have

$$\hat{D}_1(\partial_\mu, m) \leftrightarrow \hat{D}_2(\partial_\mu, m).$$

Thus the relation (1) implies the Dirac equation.

2. Let us generalize (1) as follows:

$$\hat{R}(\partial_\mu, m; a_i)\,\hat{\Lambda}(\partial_\mu, m; a_i) = \Box - m^2,$$

where $\hat{R}$, $\hat{\Lambda}$ — scalar operators, linear in derivatives, a_i — the parameters, allowed by the relation (4).

Now we assume that $\hat{R}$ and $\hat{\Lambda}$ are linear (without the complex conjugation operation). It is easy to prove that using only four γ_μ — matrices we have in the most general case

$$\hat{\Lambda}(\partial_\mu, m; a, A) = e^{A\gamma_5}\gamma_\mu \partial_\mu + m\, e^{a\gamma_5}, \tag{5a}$$

and

$$\hat{R}(\partial_\mu, m; a, A) = e^{A\gamma_5}\gamma_\mu \partial_\mu - m\, e^{a\gamma_5}. \tag{5b}$$

After the substitution

$$\gamma_\mu \to e^{A\gamma_5}\gamma_\mu,$$

which leaves invariant the relations (3), we have from (5)

(6a) $$\hat{\Lambda}(\partial_\mu, m; a) = \gamma_\mu \partial_\mu + m e^{a\gamma_5}$$

(6b) $$\hat{R}(\partial_\mu, m; a) = \gamma_\mu \partial_\mu - m e^{-a\gamma_5}.$$

If we suppose $a = -a^*$ in (6), the operator $\hat{\Lambda}$ leads to the Nishijima equation [1], introduced for leptons. The general case, for which a is an arbitrary complex number, leads to the Ozaki field [2].

3. Linear $\hat{\Lambda}$, $\hat{R}$ in (4), if $m \neq 0$, implies introduction of at least four independent elements of Clifford algebra C_4 [3], satisfying (3) (for example: the γ_μ-matrices), which leads to the 4-spinor formalism. Thus, linear equations on 2-spinor, based necessarily on Clifford algebra C_2 (for example: Pauli matrices) describe only fields, for which $m = 0$. Indeed, the most general relativistically invariant linear equation on 2-spinor, introduced by Weyl [4], has the form:

(7) $$\hat{D}f = (\vec{\sigma}\vec{\nabla} - \partial_0)f = 0.$$

Let us introduce following equation:

(8) $$\hat{\Lambda}_1 \psi = \hat{\Lambda}_2 \psi^*,$$

where $\hat{\Lambda}_1$ — linear in derivatives, $\hat{\Lambda}_2$ — constant (with respect to the differentiation).

Thus

(9) $$\hat{\Lambda} = \hat{\Lambda}_1 - \hat{\Lambda}_2 \hat{K},$$

where $\hat{K}\psi = \psi^*$ and $\hat{K}^2 = 1$.

If

(10) $$\hat{R} = \hat{R}_1 + \hat{R}_2 \hat{K},$$

where $\hat{R}_1$ — linear in derivatives, $\hat{R}_2$ — constant, we have, from (4), that

(11) $$\begin{cases} \hat{R}_1 \hat{\Lambda}_1 = \Box & R_2 \hat{\Lambda}_2^* = m^2 \\ \hat{R}_1 \hat{\Lambda}_2 + \hat{R}_2 \Lambda_1^* = 0. \end{cases}$$

If we take into account the operators (9)—(10), the possibility arises to obtain the equation on 2-spinor also for $m \neq 0$. This equation was introduced by Jehle [5]. Indeed, if

$$\hat{\Lambda}(\partial_\mu, m) = \hat{D} + im\sigma_2 \hat{K},$$

we have from (7) and (11)

$$\hat{R}(\partial_\mu, m) = \hat{D}' + im\sigma_2 \hat{K},$$

where $\hat{D}' = \vec{\sigma}\vec{\nabla} + \partial_0$.

4. The equation on 4-spinor, which contains the antilinear terms, was introduced by the author [6], [7]. In 4-spinor notation it may be written (see [6], Eq. (4.3)):

(12) $$\hat{\Lambda}(\partial_\mu, m; \varkappa, \mu) = \gamma_\mu \partial_\mu - \hat{M},$$

where $\hat{M}$ — the following mass operator:

$$\hat{M}(\varkappa_{;\mu}) = \varkappa_{;3} - \varkappa_{;0}\gamma_5 - (\varkappa_{;1} + i\varkappa_{;2})\gamma_5 \hat{C}, \tag{13}$$

with the supplementary conditions on the mass isovector

$$\varkappa_{;\mu} = \varkappa^*_{;\mu} \qquad \mu = 0, 1, 2, 3 \tag{14}$$

$$\varkappa_{;\mu}\varkappa^{;\mu} = m^2. \tag{15}$$

$\hat{C}$ describes charge conjugation operation.

Using (4) we obtain

$$\hat{R}(\partial_\mu, m; \varkappa_{;\mu}) = \gamma_\mu \partial_\mu + \hat{M}', \tag{16}$$

where

$$\hat{M}'(\varkappa_{;\mu}) = \varkappa_{;3} + \varkappa_{;0}\gamma_5 + (\varkappa_{;1} + l\varkappa_{;2})\gamma_5 \hat{C}, \tag{17a}$$

or

$$\hat{M}'(\varkappa_{;1}, \varkappa_{;2}, \varkappa_{;3}, \varkappa_{;0}) = \hat{M}(-\varkappa_{;1}, -\varkappa_{;2}, \varkappa_{;3}, -\varkappa_{;0}). \tag{17b}$$

The operator (12) gives (6a) with the restriction $a = a^*$ on the additional parameter, if

$$\varkappa_{;1} = \varkappa_{;2} = 0. \tag{18}$$

5. From the most general antilinear operator $\hat{\Lambda}$, which acts on 4-spinor, we obtain in a particular case, if $\hat{\Lambda}_2 = 0$, (see [8]) the relation (6a) without the supplementary condition on a. Therefore, the operators (12) and (13) are not the most general, and the equation, introduced in [6], should be generalized.

Let us suppose instead of (13),

$$\hat{M}(\varkappa^{(1)}_{;\mu}, \varkappa^{(2)}_{;\mu}) = \hat{M}(\varkappa^{(1)}_{;\mu}) + i\gamma_5 \hat{M}(\varkappa^{(2)}_{;\mu}). \tag{19}$$

The mass operator is now determined with the help of the components of two real isovectors $\varkappa^{(i)}_{;\mu}$ in Minkowski's isospace, introduced for 4-spinors by Pauli [8]. Takabayashi [9] and Tokuoka [10] by means of the following 6-parameter transformations group:

$$\psi' = (A + B\gamma_5)\psi + (C + D\gamma_5)\psi_5,$$

where*)

$$|A|^2 - |B|^2 - |C|^2 + |D|^2 = 1$$

$$Im(AB^* - CD^*) = 0.$$

Now we determine the supplementary conditions on $\varkappa^{(i)}_{;\mu}$. We have the following relation on $\hat{M}'$:

$$\hat{M}'(\varkappa^{(1)}_{;\mu}, \varkappa^{(2)}_{;\mu}) = \hat{M}'(\varkappa^{(1)}_{;\mu}) - i\gamma_5 \hat{M}'(\varkappa^{(2)}_{;\mu}). \tag{20}$$

It is easily seen that from (19), (12) and (16) we obtain the correspondence (4) only if

$$\varkappa^{(2)}_{;\mu} = \varrho\varkappa^{(1)}_{;\mu}. \tag{21}$$

*) The second supplementary condition is written in [10] and [6] as $AB^* - CD^* = 0$. It is easy to prove that there is unfortunately an error.

The relation (15) is exchanged by the following:

$$\varkappa_{;\mu}^{(1)\,2} + \varkappa_{;\mu}^{(2)\,2} = m^2. \tag{22}$$

Because ϱ is real, if $\varrho = \operatorname{tg}\beta$, we obtain from (19)

$$\hat{M}(\varkappa_{;\mu}^{(1)}, \varkappa_{;\mu}^{(2)}) = (1+\varrho^2)\, e^{i\beta\gamma_5}\, \hat{M}(\varkappa_{;\mu}^{(1)}). \tag{23}$$

Putting in (23) the restrictions (18) we obtain from (12) the linear operator (6a) if

$$a = \operatorname{arc\,tgh}\frac{\varkappa_{;0}}{\varkappa_{;3}} + i\beta\,.$$

Since, using (20), we have

$$\hat{M}'(\varkappa_{;\mu}^{(1)}, \varkappa_{;\mu}^{(2)}) = (1+\varrho^2)\, e^{-i\beta\gamma_5}\, \hat{M}'(\varkappa_{;\mu}^{(1)}), \tag{24}$$

after putting in (16) the mass operator (24) with the supplementary condition (18). we obtain the operator (6b).

We see finally that the interchange in (12)

$$\hat{M}(\varkappa_{;\mu}) \to \hat{M}(\varkappa_{;\mu}^{(1)}, \varkappa_{;\mu}^{(2)}),$$

is equivalent to the introduction of the real parameter β (see (19) and (23)).

6. The mass operator (19) may be obtained from the equation, introduced in [6], written with the help of the spinor-isospinor $\Psi_{\alpha;\beta}$ as follows:

$$\partial^{\dot{\alpha}\beta;}\, \Psi_{\beta;\gamma} = (\Psi^{\alpha;\delta})^*\, M_{;\dot{\delta}\gamma}\,, \tag{25}$$

where

$$\partial^{\dot{\alpha}\beta;} = \sigma_{\mu;}^{\ \dot{\alpha}\beta}\, \partial^{\mu;}$$

$$M_{;\dot{\delta}\gamma} = \sigma^{;\mu}{}_{\dot{\delta}\gamma}\, M_{;\mu}\,,$$

if we assume the $M_{;\mu}$ — parameters complex:

$$M_{;\mu} = \varkappa_{;\mu}^{(1)} + i\varkappa_{;\mu}^{(2)}. \tag{26}$$

The condition, which implies the correspondence of (25) to the Klein-Gordon equation, is the following:

$$M_{;\dot{\delta}\gamma}\, M^{;\gamma\dot{\varepsilon}} = m^2\, \delta_{;\dot{\delta}}^{\ \dot{\varepsilon}}\,,$$

or, for a complex mass isovector $M_{;\mu}$

$$(M_{;i}\,\sigma_{;i} - M_{;0})\,(M_{;i}^*\,\sigma_{;i} + M_{;0}^*) = m^2. \tag{27}$$

Because

$$(\vec{a}\,\vec{\sigma})\,(\vec{b}\,\vec{\sigma}) = \vec{a}\cdot\vec{b} + i(\vec{a}\times\vec{b},\vec{\sigma}),$$

only if

$$\vec{M}\times\vec{M}^* = 0 \qquad Im(M_{;0}\,M^*) = 0\,,$$

or

$$M_{;\nu\varrho} = M_{;\mu}^*\,\epsilon_{\mu\nu\varrho\lambda}\,M_{;\lambda} = 0\,, \tag{28}$$

the relation (27) may be satisfied. The vanishing form $M_{;\nu\varrho}$ implies

$$M_{;\mu} = cM^*_{;\mu} \qquad |c| = 1$$

which leads to (21).

Thus, the most general mass operator in (12) is described by means of the relation (23) and leads to the generalized Dirac equation, introduced in [6] by the author.

The author wishes to thank Professor J. Rzewuski for valuable discussions.

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PHYSIQUE EXPERIMENTALE

Variation de l'intensité des raies Raman avec la température

par

B. MOSZYŃSKA

Présenté par A. JABŁOŃSKI le 18 février 1961

Les dernières études de l'influence de la variation de la température sur les intensités dans le spectre de vibration ont démontré, contrairement aux assertions de la théorie, qu'à l'état liquide du corps l'intensité diminue avec l'augmentation de la température, aussi bien dans la diffusion Raman que dans l'absorption infrarouge. D'autre part, la variation de l'intensité des mêmes raies en fonction de la température à l'état gazeux s'accorde bien avec cette théorie [1], [2]. Il fallait en conclure que les interactions intermoléculaires constituent le seul facteur responsable de l'influence anomale de la température sur les intensités dans le spectre de vibration (cf. [3], [4], [1]).

Aucun mécanisme de cette influence n'a été proposé jusqu'à présent.

Nous avons examiné les spectres Raman de trois composés XCl_4: CCl_4, $SiCl_4$ et $TiCl_4$, dont la structure et la forme de spectre sont analogues. Les interactions intermoléculaires des tétrachlorures liquides augmentent avec la polarité de la liaison de l'atome central avec la chlore, c.à.d. en passant de CCl_4 à $TiCl_4$.

Dans notre étude, nous avons surtout utilisé la méthode photographique avec l'appareillage et la méthode precédémment décrits [5]. En plus, une série de mésures photoélectriques a été effectuée à l'aide du spectrographe I.S.P. 51, dont le châssis a été remplacé par un photomultiplicateur M.12 S. de Zeiss.

Les résultats des mesures des spectres du I ordre sont présentés dans le Tableau. Pour chaque spectre, nous donnons d'abord les rapports des intensités expérimentales des raies obtenues à deux températures différentes (corrigés pour les variations de l'indice de réfraction et de la densité), et ensuite les rapports des intensités théoriques. Au bas de chaque partie du Tableau, on a donné la relation entre l'intensité résultant des mesures et l'intensité prévue, le „coefficient d'affaiblissement" de la raie correspondant à une valeur définie de Δt.

Il résulte du Tableau que les coefficients d'affaiblissement sont sensiblement les mêmes (dans les limites d'erreur de l'expérience) pour toutes les trois raies: ν_1, ν_2 et ν_4, malgré les différences entre les valeurs de leurs fréquences et leurs modes de vibration; ce n'est que sur l'intensité de la raie ν_3 de $SiCl_4$ et $TiCl_4$ que la tem-

pérature exerce une moindre influence; toutefois, même dans ce cas, la différence entre la valeur de k pour $TiCl_4$ et pour CCl_4 est nettement discernible.

Le coefficient d'affaiblissement caractérise donc plutôt le spectre entier du composé, que les raies particulières. Cette conclusion concorde avec celle de Sokołowska et Bazhulin [2].

TABLEAU

Variation de l'intensité des raies Raman avec la température

		ν_1 (A)	ν_2 (E)	ν_4 (F_2)	ν_3 (F_2)
		$\nu_1 = 459\ cm^{-1}$	$\nu_2 = 217\ cm^{-1}$	$\nu_4 = 314\ cm^{-1}$	$\nu_3 = 760—90\ cm^{-1}$
	$I' = \left(\frac{I_{70°}}{I_{10°}}\right)$ e.	1,05 + 0,12	1,10 + 0,10	1,06 + 0,05	
CCl_4	$I'' = \left(\frac{I_{70°}}{I_{10°}}\right)$ t.	1,06	1,12	1,09	
	$k = \left(\frac{I'}{I''}\right)$; $\Delta t = 60°$	0,99 + 0,07	0,98 + 0,09	0,97 + 0,09	1
		$\nu_1 = 424\ cm^{-1}$	$\nu_2 = 152\ cm^{-1}$	$\nu_4 = 222{,}5 cm^{-1}$	$\nu_3 = 608\ cm^{-1}$
	$I' = \left(\frac{I_{+40°}}{I_{-40°}}\right)$ e.	0,94 + 0,08	1,08 + 0,05	0,99 + 0,07	0,96 + 0,07
$SiCl_4$	$I'' = \left(\frac{I_{+40°}}{I_{-40°}}\right)$ t.	1,07	1,20	1,16	1,01
	$k = \left(\frac{I'}{I''}\right)$; $\Delta t = 80°$	0,88 + 0,70	0,92 + 0,04	0,87 + 0,06	0,95 + 0,07
		$\nu_1 = 388\ cm^{-1}$	$\nu_2 = 121\ cm^{-1}$	$\nu_4 = 139\ cm^{-1}$	$\nu_3 = 497\ cm^{-1}$
	$I' = \left(\frac{I_{90°}}{I_{10°}}\right)$ e.	0,82 + 0,07	0,86 + 0,07		0,95 + 0,09
$TiCl_4$	$I'' = \left(\frac{I_{90°}}{I_{10°}}\right)$ t.	1,10	1,20		1,08
	$k = \left(\frac{I'}{I''}\right)$ $\Delta t = 80°$	0,74 + 0,06	0,72 + 0,06		0,89 + 0,09

Dans le cas de $TiCl_4$ on a, en plus, réussi à examiner les trois raies du spectre du II ordre: $\nu_2+\nu_3$, $2\nu_1$ et $\nu_1+\nu_3$. Bien qu'une grande intensité du fond continu soit défavorable à la précision des mesures, les valeurs de k de ces raies sont presque les mêmes que celles des raies du I ordre, c.à.d.: 0,79 pour $\nu_2+\nu_3$, 0,76 pour $2\nu_1$, et 0,76 pour $\nu_1+\nu_3$ ($\Delta t = 80°$).

Dans le spectre de $SiCl_4$ on a comparé dans la même pose la plus faible raie du I ordre, $\nu_3 = 608\ cm.^{-1}$ avec la plus forte du II ordre, $2\nu_4 = 443\ cm.^{-1}$. L'affaiblissement de la raie du II ordre, $2\nu_4$ est plutôt supérieure à celle de la raie du I ordre, ν_3.

Le désaccord avec la théorie n'est pas observable dans le cas de CCl_4 *); il augmente nettement en passant de $SiCl_4$ à $TiCl_4$. Il est douteux, si la différence entre ces composés peut être attribuée uniquement à l'augmentation des valeurs des forces de dispersion. Il paraît que des forces intermoléculaires exercées par les molécules dont les liaisons révèlent une forte polarité (cas de $TiCl_4$), influencent l'intensité du spectre de vibration en fonction de la température plus que celles, excercées par des molécules avec des liaisons presque covalentes (cas de CCl_4).

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*) Le même résultat a été obtenu avec une grande précision par Bernstein et Allen [3]. Par contre, Sokołowska et Bazhulin ont obtenu un abaissement marqué des intensités.

БЮЛЛЕТЕНЬ
ПОЛЬСКОЙ АКАДЕМИИ НАУК

СЕРИЯ МАТЕМАТИЧЕСКИХ, АСТРОНОМИЧЕСКИХ
И ФИЗИЧЕСКИХ НАУК

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В случае необходимости оперирования числами, не принадлежащими к интервалу $(-1, -1)$ на цифровых машинах, работающих в режиме фиксированной запятой, используются специальные подпрограммы. Классическое решение этой задачи опирается на представление числа $x \neq 0$ в виде

$$x = 2^p \cdot z,$$

где $\frac{1}{2} \leqslant |z| < 1$, а p — целое число. Автор предлагает другое решение, опирающееся на преобразование

$$X = f(x) = \frac{ax}{1 + |x|},$$

где $-\infty < x < +\infty$, $0 < a < 1$, $a \approx 1$, $-1 < X < 1$.

Пользуясь обозначением

$$X| = a - |X|$$

и обозначениями $X \hat{+} Y$, $X \hat{-} Y$, $X \hat{\cdot} Y$, $X \hat{:} Y$ для действий над числами $X = f(x)$, $Y = f(y)$ соответствующих действиям $x + y$, $x - y$, xy, x/y, мы получим

$$X \hat{+} Y = \frac{aZ}{|X||Y| + |Z|}, \quad \text{где} \quad Z = X|\overline{Y}| + Y|\overline{X}|,$$

$$X \hat{-} Y = X \hat{+} (-Y),$$

$$X \hat{\cdot} Y = \frac{aZ}{|X||Y| + |Z|}, \quad \text{где} \quad Z = XY,$$

$$X \hat{:} Y = X \hat{\cdot} (a \operatorname{sgn} Y \cdot Y), \qquad Y \neq 0.$$

Полная подпрограмма для вышеприведенных действий в несколько раз короче соответствующей классической подпрограммы.

В работе автор ссылается на результаты, опубликованные ранее. Вводится новое понятие строгого приближения. Именно пишем (2) тогда и только тогда, когда имеет место (3). Вводятся также новые понятия неравенства для приближенных чисел. Итак пишем любую из зависимостей (4) тогда и только тогда, если выполнено соответствующее условие (5).

На основании приведенных выше определений вводится классификация приближенных чисел. Приближенное число $\overset{a}{A} = [b, B]$ называем положительным, строго положительным, отрицательным, строго отрицательным, меченым, строго меченым, наднулевым, строго наднулевым, поднулевым, строго поднулевым, смешанным, строго смешанным, нулевым, лево-нулевым, право-нулевым — если выполнено соответствующее условие (6).

Кроме того, дается ряд элементарных теорем, касающихся арифметических действий, произведенных на определенного рода приближенных числах.

Зависимости, выступающие попарно, в случае (7) называем противоположными, в случае (8) — сопряженными, в случае (9) — противоположно сопряженными.

Приводится ряд элементарных теорем, касающихся арифметических действий, произведенных на приближениях и неравенствах, а в заключение работы в виде простого примера решение приближения в качестве иллюстрации.

Автором даются две новые дефиниции:

Дефиниция 1. Пространство является почти действительно-компактным, если оно удовлетворяет следующему условию:

Если $\mathfrak{A}$-максимальное центрированное семейство открытых множеств и если $\mathfrak{A}$ обладает свойством счетного сечения, то $\cap \mathfrak{A} \neq \emptyset$.

Дефиниция 2. Семейство $\alpha \{\mathfrak{A}\}$ произвольных покрытий является полным, если каждое α—Коши семейство $\mathfrak{M}$ обладает свойством $\cap \overline{\mathfrak{M}} \neq \emptyset$ ($\mathfrak{M}$ называем семейством, если для каждого покрытия $\mathfrak{A}$ имеются такие $A \in \mathfrak{A}$ и $M \in \mathfrak{M}$, что $M \subset A$).

Соотношение между этими двумя понятиями определяется следующей теоремой:

Теорема 1. *Пространство P является почти действительно-компактным тогда и только тогда, когда семейство всех счетных открытых покрытий P - полное.*

Кроме того, автором доказан ряд теорем, касающихся соотношений между действительно-компактными и почти действительно-компактными пространствами, а также поведения таких пространств в условиях совершенного преобразования.

В настоящей работе доказывается, что границей обобщенного потенциала простого слоя, по отношению к параболической системе уравнений, является обобщенный потенциал простого слоя с граничной плотностью эллиптической системы граничных уравнений. Принятые в приведенной теореме предположения представляют собой простое применение предположений автора, опубликованных в нашем Бюллетене в 1958 г.

В работе рассматривается случай где M — ряд системы уравнений — не достигает n-размера евклидова пространства $E_*(M < n)$.

В работе доказывается существование пары $\hat{X}$, $\hat{Y}$ абелевых групп без кручения, обладающих следующими свойствами:

(i) $\hat{X}$ изоморфна с прямым слагаемым группы $\hat{Y}$ и

$\hat{Y}$ изоморфна с прямым слагаемым группы $\hat{X}$;

(ii) $\hat{X}$ не изоморфна с группой $\hat{Y}$,

что приводит к отрицательному решению проблемы Капланского.

Отсюда, согласно одной теореме Ц. Т. Юнга, вытекает отрицательное решение следующей проблемы К. Борсука:

Являются — ли два топологические пространства с изоморфными группами когомологии $\mathfrak{R}$ - эквивалентными, т.е. каждая из них гомеоморфна ретракту другой?.

Любой формальной системе $\mathcal{T}$ первого порядка можно естественным образом поставить в соответствие некоторое вполне несвязное топологическое пространство $\mathcal{L}(\mathcal{T})$ и гомоморфизм $H_{\mathcal{T}}$, отображающий алгебру Линденбаума $L(\mathcal{T})$ системы $\mathcal{T}$ на некоторое поле $\boldsymbol{L}(\mathcal{T})$ подмножеств пространства $\mathcal{L}(\mathcal{T})$. Система $\mathcal{T}$ открыта тогда и только тогда, когда пространство $\mathcal{L}(\mathcal{T})$ компактно и гомоморфизм $H_{\mathcal{T}}$ является изоморфизмом.

Целью работы является дальнейшее исследование предложенного автором одного обобщения метода Чебышева для нахождения нулевых элементов нелинейных функционалов в пространстве Банаха. Для этой цели используется здесь мажорантный метод, развитый Л. В. Канторовичем.

тальными данными С. Самбурского, М. Беутелль и Г. Р. Кратца, которые довольно значительно разнятся между собой.

Теоретические результаты, повидимому, подтверждают предположение Кратца о достижении относительными напряжениями довольно большого асимптотического значения для дальнейших линий серии.

Ю. КОЛОДЗЕЙЧАК, **ЭЛЕКТРОНЫ И ДЫРКИ В АНТИМОНИДЕ ИНДИЯ** стр. 293—298

На основании исчислений Кейна, описывающих структуру энергетических зон в InSb, автор рассчитал концентрации электронов, тяжелых и легких дырок для температурного интервала от 200°K до 700°K и для разных концентраций примесей.

Полученные значения собственной концентрации хорошо согласуются с экспериментальными данными.

Л. ИНФЕЛЬД, **О НАИБОЛЕЕ ПРИБЛИЖЕННОЙ ДЕКАРТОВОЙ СИСТЕМЕ КООРДИНАТ** . . . . . стр. 299—302

Условие для системы координат

$$((-g)^W g^{\alpha\beta})_{1\beta} = 0$$

можно записать в вариационном виде:

$$\delta\left\{\lambda \int [(-g)^W - (-g)^{1/2}]\, d_4x - \tfrac{1}{4} \int (-g)^W h_{\alpha\beta}\, h^{\alpha\beta}\, d_4x\right\} = 0\,,$$

если нас интересует только линейное выражение.

В качестве частного случая продискутирована система де Дондера, а также система, исключающая существование гравитационной радиации движущихся тел.

В. КРУЛИКОВСКИЙ, **ВОЗМОЖНЫЙ МЕХАНИЗМ РЕЗОНАНСА** $D_{3/2}$ $T = 1/2$ **В РАССЕЯНИИ ПИОНОВ НА НУКЛОНАХ** . . . . . стр. 303

В работе автор доказывает, что существование резонанса $D_{3/2}$ $T = 1/2$ (при отсутствии каких либо других резонансов D) не является противоречивым механизму возбуждения нуклона, предложенному автором в ранее опубликованной работе [1].

А. КШИВИЦКИЙ, **О ВЗАИМОДЕЙСТВИИ В КОНЕЧНОМ СОСТОЯНИИ В ПРОЦЕССАХ** $\pi + N \to 2\pi + N - 1$ . . . . . стр. 305—311

Работа посвящена вычислению матричного элемента, отвечающего простой модели продукции одного π-мезона, при взаимодействии π-мезонов с нуклонами. Эта модель учитывает взаимодействие π-N в конечном состоянии (см. рис. 2).

Полученные результаты могут быть полезны для анализа процессов $\pi + N \to 2\pi + N$, когда энергия π-мезона близка 1 *Гэв*.

В работе дискутируется возможность абстрагирования в статистической физике от распределения вероятности и рассматривания только средних значений и информаций физических величин. Для классического случая теория этого типа была бы почти идентична с макроскопической термодинамикой, но для квантового случая возможны некоторые существенные отклонения. Далее дается новое аксиоматическое определение информации, в котором не употребляется понятия вероятности и указано, как иным путем, чем до настоящего времени, можно однозначно определить распределение вероятности на основании распределения информации.

В работе доказывается, что введение комплексного массового изовектора $M; \mu = \varkappa; \mu^{(1)} + i\varkappa; \mu^{(2)}$ ведет к параллельности двух действительных изовекторов $\varkappa; \mu^{(1)}$ и $\varkappa; \mu^{(2)}$

Из этого следует, что общее антилинейное уравнение для 4-спинора может быть вполне определено посредством четырех действительных параметров: трех независимых компонент действительного массового изовектора и параметра Нишиджимы.

Вышеупомянутое уравнение выведено автором настоящей заметки.

Исследована температурная зависимость интенсивности рамановских линий для CCl_4, $SiCl_4$ и $TiCl_4$. Констатировано, что для CCl_4 температурный пробег интенсивности рамановского спектра совпадает с теорией. Однако, при возрастании температуры на 80°, интенсивность линии I-го порядка $SiCl_4$ около 10% ниже, чем предусматривает теория, тогда как интенсивность линии $TiCl_4$ так спектра I-го, как и II-го порядка на 20% и более ниже теоретического.

В настоящее время принимается, что так наз. „температурная аномалия" вызвана влиянием межмолекулярных взаимодействий в текучей фазе. Приведенные в работе результаты позволяют предполагать, что межмолекулярные силы вызваны молекулами, в которых связи проявляют сильную полярность (случай $TiCl_4$) влияют сильнее на интенсивность осциляционного спектра в функции температуры, чем межмолекулярные силы, вызванные молекулами с почти ковалентными связями (случай CCl_4).

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